| Ref<br># | Hits | Search Query  | DBs   | Default<br>Operator | Plurals          | Time Stamp       |
|----------|------|---|---|---------------------|------------------|------------------|
| L1       | 0    | 7,7-diphenyl-2,4,6-heptatrienoic                                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR                  | OFF              | 2006/04/13 06:32 |
| L2       | 0    | (Histone adj deacetylase) and (("562/495").CCLS.)               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR                  | OFF              | 2006/04/13 06:32 |
| L3       | 0    | ("I7andI17").PN.  | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L4       | 0    | heptatrieno\$ and (("562/491").CCLS.)                           | USPAT;<br>EPO; JPO;<br>DERWENT              | OR                  | OFF              | 2006/04/13 06:32 |
| L5       | . 0  | 0 heptatrien\$ and (("562/491").CCLS.) USPAT; EPO; JPO; DERWENT |   | OFF                 | 2006/04/13 06:32 |                  |
| L6       | 0    | (dodecen\$ and insecticid\$) and "2005271"                      | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR                  | ON               | 2006/04/13 06:32 |
| L7       | 288  | (514/559).CCLS.   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L8       | 927  | (514/562).CCLS.   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L9       | 437  | (514/564).CCLS.   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L10      | 739  | (514/570).CCLS.   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L11      | 186  | (514/571).CCLS.   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR                  | OFF              | 2006/04/13 06:32 |
| L12      | . 0  | 7,7-diphenyl-2,4,6-heptatrienoic                                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR                  | OFF              | 2006/04/13 06:32 |
| L13      | 0    | (Histone adj deacetylase) and (("562/495").CCLS.)               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR                  | OFF              | 2006/04/13 06:32 |

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|-----|---------------------------------------|--|---|----|-------|------------------|
| L14 | 0                                     | ("I7andI17").PN.                           | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF   | 2006/04/13 06:32 |
| L15 | 0                                     | heptatrieno\$ and (("562/491").CCLS.)      | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |
| L16 | 0                                     | heptatrien\$ and (("562/491").CCLS.)       | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |
| L17 | 0                                     | (dodecen\$ and insecticid\$) and "2005271" | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON    | 2006/04/13 06:32 |
| L18 | 288                                   | (514/559).CCLS.                            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF   | 2006/04/13 06:32 |
| L19 | 927                                   | (514/562).CCLS.                            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF   | 2006/04/13 06:32 |
| L20 | 437                                   | (514/564).CCLS.                            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF . | 2006/04/13 06:32 |
| L21 | 739                                   | (514/570).CCLS.                            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF   | 2006/04/13 06:32 |
| L22 | 186                                   | (514/571).CCLS.                            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF   | 2006/04/13 06:32 |
| L23 | 1                                     | heptatrienoic and histone                  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |
| L24 | 1                                     | 7-phenyl-2,4,6-heptatrienoic               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |
| L25 | 1                                     | histone and heptatrieno\$                  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |
| L26 | 1                                     | "4621099".URPN.                            | USPAT                                       | OR | ON    | 2006/04/13 06:32 |
| L27 | 1                                     | heptatrienoic and histone                  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF   | 2006/04/13 06:32 |

| L28 | 1  | 7-phenyl-2,4,6-heptatrienoic             | USPAT;<br>EPO; JPO;                         | OR   | OFF | 2006/04/13 06:32 |
|-----|----|--|---|------|-----|------------------|
|     |    |  | DERWENT                                     |      |     |                  |
| L29 | 1  | histone and heptatrieno\$                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L30 | 1  | "4621099".URPN.                          | USPAT                                       | OR   | ON  | 2006/04/13 06:32 |
| L31 | 2  | ("4663336").PN.                          | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | OFF | 2006/04/13 06:32 |
| L32 | 2  | "53101527".pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L33 | 78 | heptatrieno\$                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L34 | 71 | (Histone adj deacetylase) and hydroxamic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR · | OFF | 2006/04/13 06:32 |
| L35 | 3  | "2001038322".pn.                         | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L36 | 3  | "9814424".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L37 | 53 | heptatrienoic                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L38 | 3  | 7-phenyl-2,4,6-heptatrieno\$             | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L39 | 2  | "5037813".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L40 | 2  | "4371516".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L41 | 2  | "4371516".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L42 | 16 | "2005271"                                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |

| L43 | 2  | "5747537".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
|-----|----|--|---|------|-----|------------------|
| L44 | 3  | "9929640".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L45 | 2  | "53101527".pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L46 | 2  | "9827162".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L47 | 2  | "4810299".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L48 | 2  | "4621099".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR . | ON  | 2006/04/13 06:32 |
| L49 | 2  | "5459149".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L50 | 5  | "2849466" .pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L51 | 2  | "53101527".pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L52 | 78 | heptatrieno\$                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L53 | 71 | (Histone adj deacetylase) and hydroxamic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR . | OFF | 2006/04/13 06:32 |
| L54 | 3  | "2001038322".pn.                         | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L55 | 3  | "9814424".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |

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|-----|----|------------------------------|---|---------|-----|------------------|
| L56 | 53 | heptatrienoic                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR      | OFF | 2006/04/13 06:32 |
| L57 | 3  | 7-phenyl-2,4,6-heptatrieno\$ | USPAT;<br>EPO; JPO;<br>DERWENT              | ÓR      | OFF | 2006/04/13 06:32 |
| L58 | 2  | "5037813".pn.                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR      | OFF | 2006/04/13 06:32 |
| L59 | 2  | "4371516".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR<br>· | ON  | 2006/04/13 06:32 |
| L60 | 2  | "4371516".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L61 | 16 | "2005271"                    | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L62 | 2  | "5747537".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L63 | 3  | "9929640".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR .    | ON  | 2006/04/13 06:32 |
| L64 | 2  | "53101527".pn.               | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L65 | 2  | "9827162".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L66 | 2  | "4810299".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L67 | 2  | "4621099".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |
| L68 | 2  | "5459149".pn.                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR      | ON  | 2006/04/13 06:32 |

| L69 | 5     | "2849466" .pn.             | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
|-----|-------|----------------------------|---|----|-----|------------------|
| L70 | 111   | oxamflatin                 | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L71 | 242   | (562/491).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L72 | . 242 | (562/491).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L73 | 325   | (562/495).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L74 | 325   | (562/495).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L75 | 339   | \$pentynoic                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L76 | 472   | dodecen\$ and insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L77 | 472   | dodecen\$ and insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L78 | 585   | heptatrien\$               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L79 | 585   | heptatrien\$               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L80 | 690   | Histone adj deacetylase    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L81 | 690   | Histone adj deacetylase    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |

| L82 | 6662  | hydroxamic  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
|-----|-------|---|---|----|-----|------------------|
| L83 | 4516  | histone   | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L84 | 17123 | dodecen\$   | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L85 | 75914 | insecticid\$                                      | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L86 | 6662  | hydroxamic  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L87 | 4516  | histone   | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L88 | 17123 | dodecen\$   | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L89 | 75914 | insecticid\$                                      | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | QR | ON  | 2006/04/13 06:32 |
| L90 | 2     | ("6720445").PN.                                   | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | OFF | 2006/04/13 06:32 |
| L91 | 0     | 7,7-diphenyl-2,4,6-heptatrienoic                  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L92 | 0     | (Histone adj deacetylase) and (("562/495").CCLS.) | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L93 | 0     | ("I7andi17").PN.                                  | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L94 | 0     | heptatrieno\$ and (("562/491").CCLS.)             | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L95 | 0     | heptatrien\$ and (("562/491").CCLS.)              | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |

| L96  | 0   | (dodecen\$ and insecticid\$) and "2005271"        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
|------|-----|---|---|----|-----|------------------|
| L97  | 288 | (514/559).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L98  | 927 | (514/562).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L99  | 437 | (514/564).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L100 | 739 | (514/570).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L101 | 186 | (514/571).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L102 | 0   | 7,7-diphenyl-2,4,6-heptatrienoic                  | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L103 | 0   | (Histone adj deacetylase) and (("562/495").CCLS.) | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L104 | 0   | ("I7andI17").PN.                                  | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L105 | 0   | heptatrieno\$ and (("562/491").CCLS.)             | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L106 | 0   | heptatrien\$ and (("562/491").CCLS.)              | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L107 | 0   | (dodecen\$ and insecticid\$) and "2005271"        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L108 | 288 | (514/559).CCLS.                                   | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |

|      | 1   |                              |   | 1    |     |                  |
|------|-----|------------------------------|---|------|-----|------------------|
| L109 | 927 | (514/562).CCLS.              | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR   | OFF | 2006/04/13 06:32 |
| L110 | 437 | (514/564).CCLS.              | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR   | OFF | 2006/04/13 06:32 |
| L111 | 739 | (514/570).CCLS.              | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR   | OFF | 2006/04/13 06:32 |
| L112 | 186 | (514/571).CCLS.              | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR   | OFF | 2006/04/13 06:32 |
| L113 | 1   | heptatrienoic and histone    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L114 | 1   | 7-phenyl-2,4,6-heptatrienoic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L115 | 1   | histone and heptatrieno\$    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L116 | 1   | "4621099".URPN.              | USPAT                                       | OR   | ON  | 2006/04/13 06:32 |
| L117 | 1   | heptatrienoic and histone    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L118 | 1   | 7-phenyl-2,4,6-heptatrienoic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L119 | 1   | histone and heptatrieno\$    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L120 | 1   | "4621099".URPN.              | USPAT                                       | OR   | ON  | 2006/04/13 06:32 |
| L121 | 2   | ("4663336").PN.              | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | OFF | 2006/04/13 06:32 |
| L122 | 2   | "53101527".pn.               | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR . | ON  | 2006/04/13 06:32 |
| L123 | 78  | heptatrieno\$                | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |

| L124 | 71 | (Histone adj deacetylase) and hydroxamic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR · | OFF | 2006/04/13 06:32 |
|------|----|--|---|------|-----|------------------|
| L125 | 3  | "2001038322".pn.                         | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L126 | 3  | "981 <del>44</del> 24".pn.               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L127 | 53 | heptatrienoic                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L128 | 3  | 7-phenyl-2,4,6-heptatrieno\$             | USPAT;<br>EPO; JPO;<br>DERWENT              | OR . | OFF | 2006/04/13 06:32 |
| L129 | 2  | "5037813".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:32 |
| L130 | 2  | "4371516".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L131 | 2  | "4371516".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L132 | 16 | "2005271"<br>·                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L133 | 2  | "5747537".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L134 | 3  | "9929640".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L135 | 2  | "53101527".pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |
| L136 | 2  | "9827162".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:32 |

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|------|----|--|---|----|-----|------------------|
| L137 | 2  | "4810299".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L138 | 2  | "4621099".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L139 | 2  | "5459149".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L140 | 5  | "2849466" .pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L141 | 2  | "53101527".pn.                           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L142 | 78 | heptatrieno\$                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L143 | 71 | (Histone adj deacetylase) and hydroxamic | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L144 | 3  | "2001038322".pn.                         | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L145 | 3  | "9814424".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L146 | 53 | heptatrienoic                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L147 | 3  | 7-phenyl-2,4,6-heptatrieno\$             | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L148 | 2  | "5037813".pn.                            | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L149 | 2  | "4371516".pn.                            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |

|      | ı          | T                    |   |    |     | <del></del>      |
|------|------------|----------------------|---|----|-----|------------------|
| L150 | 2          | "4371516".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L151 | 16         | "2005271"            | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L152 | 2          | "5747537".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L153 | 3          | "9929640".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L154 | 2          | "53101527".pn.       | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L155 | 2          | "9827162".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L156 | 2          | "4810299".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L157 | 2          | "4621099".pn.        | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L158 | 2          | <b>"5459149".pn.</b> | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L159 | 5          | "2849466" .pn.       | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L160 | <b>111</b> | oxamflatin           | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L161 | 242        | (562/491).CCLS.      | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |

| L162 | 242   | (562/491).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
|------|-------|----------------------------|---|----|-----|------------------|
| L163 | 325   | (562/495).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L164 | 325   | (562/495).CCLS.            | USPAT;<br>USOCR;<br>EPO; JPO;<br>DERWENT    | OR | OFF | 2006/04/13 06:32 |
| L165 | 339   | \$pentynoic                | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L166 | 472   | dodecen\$ and insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L167 | 472   | dodecen\$ and insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:32 |
| L168 | 585   | heptatrien\$               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L169 | 585   | heptatrien\$               | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L170 | 690   | Histone adj deacetylase    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L171 | 690   | Histone adj deacetylase    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L172 | 6662  | hydroxamic                 | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:32 |
| L173 | 4516  | histone                    | USPAT;<br>EPO; JPO;<br>DERWENT              | OR | OFF | 2006/04/13 06:33 |
| L174 | 17123 | dodecen\$                  | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR | ON  | 2006/04/13 06:33 |

| L175 | 75914 | insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:33 |
|------|-------|--------------|---|------|-----|------------------|
| L176 | 6662  | hydroxamic   | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:33 |
| L177 | 4516  | histone      | USPAT;<br>EPO; JPO;<br>DERWENT              | OR   | OFF | 2006/04/13 06:33 |
| L178 | 17123 | dodecen\$    | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR   | ON  | 2006/04/13 06:33 |
| L179 | 75914 | insecticid\$ | US-PGPUB;<br>USPAT;<br>EPO; JPO;<br>DERWENT | OR . | ON  | 2006/04/13 06:33 |

4/13/06 6:53:19 AM
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Page 14

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USPAT2
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NEWS 7 JAN 17 IPC 8 in the WPI family of databases including WPIFV

NEWS 8 JAN 30 Saved answer limit increased

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NEWS 17 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes.

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NEWS 19 MAR 22 EMBASE is now updated on a daily basis

NEWS 20 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL

NEWS 21 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL

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\* effective March 20, 2005. A new display format, IDERL, is now \* \* effective March 20, 2005. A new display format, IDERL, is now 

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Structure search iteration limits have been increased. See HELP SLIMITS or details. പട്ടുകളുടെ നിന്നു പട്ടു വിശ്യാന് അതിന്റെ അതിന്റെ വിവര് വിവര് വിശ്യാത്ത് വിശ്യാത്ത് വിശ്യാത്ത് വിശ്യാത്ത് വിശ്യാ

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=> e 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI METHYLPHENYL) -3,7-DIMETHYL-, ETHYL ESTER, (ALL-E)-/CN E1 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, ETHYL ESTER/ E2 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, METHYL ESTER /CN E3 0 --> 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI METHYLPHENYL) -3,7-DIMETHYL-, ETHYL ESTER, (ALL-E)-/CN2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI F.4 1 METHYLPHENYL)-3,7-DIMETHYL-, ETHYL ESTER, (ALL-E)-/CN 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI E.5 1 METHYLPHENYL)-3,7-DIMETHYL-, ETHYL ESTER, (Z,E,E,E)-/CN E6 1 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI METHYLPHENYL) -3,7-DIMETHYL-, ETHYL ESTER, (Z,E,E,Z)-/CN E7 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,5-DIMET HYL-1,3-CYCLOHEXADIEN-1-YL)-3,7-DIMETHYL-, ETHYL ESTER, (ALL -E)-/CN

| E8    | 1 | 2,4,6,8-NONATETRAENOIC ACID, 2-METHOXY-9-PHENYL-, ETHYL ESTE R/CN  |
|-------|---|--|
| E9    | 1 | 2,4,6,8-NONATETRAENOIC ACID, 2-METHYL-9-PHENYL-, METHYL ESTE R, (2E,4E,6E,8E)-/CN                              |
| E10   | 1 | 2,4,6,8-NONATETRAENOIC ACID, 2-METHYL-9-PHENYL-, METHYL ESTE R, (ALL-E)-/CN                                    |
| E11   | 1 | 2,4,6,8-NONATETRAENOIC ACID, 3,7-DIETHYL-9-(2-(HEXYLOXY) PHEN YL)-, (ALL-E)-/CN                                |
| E12   | 1 | 2,4,6,8-NONATETRAENOIC ACID, 3,7-DIETHYL-9-(2-NAPHTHALENYL)-, ETHYL ESTER/CN                                   |
| => e4 |   |  |
| L1    |   | 4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRIMET PHENYL)-3,7-DIMETHYL-, ETHYL ESTER, (ALL-E)-"/CN |

=> d 11

ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 71184-23-1 REGISTRY

CN 2,4,6,8-Nonatetraenoic acid, 2-fluoro-9-(4-methoxy-2,3,6-

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MF C23 H29 F O3

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ANSWER 1 OF 2. CAPLUS COPYRIGHT 2006 ACS on STN

TI Effects of carcinogens and retinoids on prostatic explants

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Effects of carcinogens and retinoids on prostatic explants

AU Chopra, D. P.; Wilkoff, L. J.

CS. Cell Biol. Div., South. Res. Inst., Birmingham, AL, 35205, USA

SO Clin. Androl. (1981), Volume 6, Issue Prostatic Carcinoma: Biol. Diagn.,
166-74 Editor(s): Hafez, E. S. E.; Spring-Mills, E. Publisher: Nijhoff, The Hague, Neth.

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CODEN: 47GVAQ

DT Conference

LA SEnglish was to be a second or the second of the second

- AB Culture methods for mouse prostate explants are discussed along with the and the control of t effects of various carcinogens on such explants. Mouse prostate explants were treated with benzo(a)pyrene [50-32-8] for 8 days and various retinoids were tested for their ability to reduce the carcinogenicity of [71407-30-2], The methylketocyclopentyl analog of retinoic acid this compound 13-cis-retinoic acid [4759-48-2], N-retinoylglycine [71407-30-2], The methylketocyclopentyl analog of retinoic acid
  [50890-42-1], the 1-methoxyethylcyclopentenyl analog of retinoic acid
  [71202-59-0], and the 14-fluoro derivative of the trimethylmethoxyphenyl analog of retinoic acid Et ester [71184-23-1] were all more active than  $\beta$ -retinoic acid [302-79-4]. Seven other retinoids had activities equal to that of  $\beta$ -retinoic acid.
  - IT Prostate gland

(explants, retinoids as neoplasm inhibitors in)

IT Neoplasm inhibitors

(retinoids as)

302-79-4 1671-98-3 3887-00-1 4759-48-2 10035-29-7 32450-56-9 IT 50890-42-1 54350-48-0 58970-49-3 63700-89-0 63826-42-6 69877-53-8 **71184-23-1** 71202-59-0 71407-30-2 81425-66-3 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(as neoplasm inhibitor)

TΨ 50-32-8, biological studies

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study) (carcinogenicity of, retinoids effect on)

- L2 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Fluorinated retinoic acids and their analogs. 1. Synthesis and biological activity of (4-methoxy-2,3,6-trimethylphenyl)nonatetraenoic acid analogs
- 1979:517154 CAPLUS AN

DN 91:117154

- TI Fluorinated retinoic acids and their analogs. 1. Synthesis and biological activity of (4-methoxy-2,3,6-trimethylphenyl)nonatetraenoic acid analogs
- Pawson, Beverly A.; Chan, Ka-Kong; DeNoble, James; Han, Ru Jen L.; AU Piermattie, Virginia; Specian, Anthony C.; Srisethnil, Srisamorn; Trown, Patrick W.; Bohoslawec, Oksana; et al.
- Chem. Res. Dep., Hoffmann-La Roche Inc., Nutley, NJ, 07110, USA CS
- Journal of Medicinal Chemistry (1979), 22(9), 1059-67 SO CODEN: JMCMAR; ISSN: 0022-2623
- DT
- LA English

GI

The title compds. were prepared and evaluated for their therapeutic effect AB on chemical-induced skin papillomas in mice. The hypervitaminosis A dose, a measure of toxicity, was also determined A therapeutic effect greater than that of the parent nonfluorinated ester was shown by I [3887-00-1], (II). [63700-90-3], (III) [63651-02-5], (IV) [69877-58-3], (V) [71145-31-8], and (VI) [71184-25-3]. Substitution of F for H at C-4 or C-6 in the aromatic series had the greatest pos. effect on antipapilloma activity. Structure-activity relations are discussed.

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ΙT Neoplasm inhibitors

(fluororetinoids)

- IT Molecular structure-biological activity relationship (neoplasm-inhibiting, of fluororetinoids)
- IT 54344-92-2
  - RL: RCT (Reactant); RACT (Reactant or reagent) (Grignard reaction of)
- IT 24490-03-7
  - RL: RCT (Reactant); RACT (Reactant or reagent) (bromination of)
- IT 5927-18-4
  - RL: BIOL (Biological study)

(condensation of, with butenone derivative)

- IT
  - RL: BIOL (Biological study)

(condensation of, with fluorophosphonoacetate)

- IT 54344-92-2
  - RL: BIOL (Biological study)

(condensation of, with fluorophosphonoacetates)

IT 867-13-0

RL: BIOL (Biological study)

```
(condensation of, with octatrienone derivative)
                 IT
                         13844-35-4
                         RL: BIOL (Biological study)
                              (condensation of, with phenylpentadienal derivative)
                         54757-47-0
                 IT
                         RL: BIOL (Biological study)
                              (condensation of, with phosphonoacetates)
                 IT
                         RL: BAC (Biological activity or effector, except adverse); BSU (Biological
                         study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES
                              (neoplasm-inhibiting activity of)
                 IT
                         63651-12-7P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                              (preparation and Meyer-Schuster rearrangement of)
                 TT
                         69877-48-1P
                                               71145-26-1P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                (preparation and Wittig reaction of).
                      63651-25-2P
(preparation and condensation with phosphoacetate)
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                        RL: SPN (Synthetic preparation); PREP (Preparation)
                (preparation; and condensation with phosphonoacetate)
 IT 69877-41-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
                              (preparation and condensation with tri-Et phosphonoacetate)
IT 69877-44-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
                                                                                                                            <del>er fillet trest Committeet jagein in der feste lieft der mendette kanz is er te</del>nte er bis der fille
                       (preparation and conversion to acetal)
                 IT
                         69877-50-5P
                                              69877-51-6P
                        RL: SPN (Synthetic preparation); PREP (Preparation)
                              (preparation and conversion to esters)
                         69877-54-9P
                 ΙT
                        RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                                                                                         (preparation and fluorination of)
                 IT
                         26586-02-7P
                                               63651-18-3P 63651-21-8P
                                                                                           63651-22-9P 63673-31-4P
                         69877-62-9P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                              (preparation and hydrolysis of)
                 IT
                         63651-17-2P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                              (preparation and isomerization of)
                 IT
                         2609-26-9P
                                             3887-00-1P 63651-02-5P
                                                                                        63700-90-3P
                                                                                                              69877-58-3P
                                              71145-31-8P 71184-25-3P
                         69877-66-3P
                        RL: BAC (Biological activity or effector, except adverse); BSU (Biological
                         study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
                         BIOL (Biological study); PREP (Preparation); USES (Uses)
                              (preparation and neoplasm-inhibiting activity of)
                 IT
                         63650-98-6P 63650-99-7P
                                                                     63651-06-9P 63651-07-0P
                                                                                                                 63651-15-0P
                         63651-38-7P
                                              71145-25-0P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                              (preparation and oxidation of)
                 IT
                         69877-38-9P
                                              69877-39-0P
                         RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
                         (Reactant or reagent)
                              (preparation and reaction with C5 fluorophosphonates)
```

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IT
               63651-16-1P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
               (Reactant or reagent)
                  (preparation and reaction with C5 phosphonate)
          IT
               63651-28-5P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
               (Reactant or reagent)
                  (preparation and reaction with fluorophosphonate derivative)
          IT
                            63651-23-0P 63651-24-1P
                                                      69877-64-1P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
               (Reactant or reagent)
                  (preparation and reaction with methyllithium)
          IT
               63758-07-6P
                            69877-43-6P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
               (Reactant or reagent)
                  (preparation and reaction with phenylpentadienal derivative)
          IT
               63651-08-1P
                            63651-09-2P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
               (Reactant or reagent)
         (preparation and reaction with phosphonate derivs.)
               69877-65-2P
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               (Reactant or reagent)
                  (preparation and reaction with phosphonoacetate)
          IT
               54344-93-3P
  RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
  (Reactant or reagent)
  with phosphorus tribromide)
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               63650-96-4P
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               69877-42-5P
                            69877-46-9P
               RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
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               RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
                  (preparation and spectra of)
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               63651-29-6P
               RL: SPN (Synthetic preparation); PREP (Preparation)
                  (preparation of)
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               71145-27-2
               RL: RCT (Reactant); RACT (Reactant or reagent)
                  (reaction of, with aldehyde derivative)
          IT
               63826-41-5
               RL: RCT (Reactant); RACT (Reactant or reagent)
                  (reaction of, with fluorophosphonate derivative)
          IT
                           2609-24-7
               RL: RCT (Reactant); RACT (Reactant or reagent)
                  (reaction of, with phenylpentadienal derivative)
          IT
               RL: RCT (Reactant); RACT (Reactant or reagent)
                  (reaction of, with phenylpentadienal derivs.)
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               54344-92-2
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RL: RCT (Reactant); RACT (Reactant or reagent)
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FILE 'REGISTRY' ENTERED AT 10:57:52 ON 12 APR 2006

E 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI
L1 1 E4

FILE 'CAPLUS' ENTERED AT 10:59:25 ON 12 APR 2006 L2 2 L1

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| => e e1 |     |   |
|---------|-----|---|
| E1      | . 1 | 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, (ALL-E)-/CN           |
| E2      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, BUTYL ESTER/          |
|         |     | CN  |
| E3      | 1>  | 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, ETHYL ESTER/          |
|         |     | CN  |
| E4      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, METHYL ESTER          |
|         |     | /CN   |
| E5      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI          |
|         |     | METHYLPHENYL) -3,7-DIMETHYL-, ETHYL ESTER, (ALL-E)-/CN                |
| E6      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI          |
|         |     | METHYLPHENYL) -3,7-DIMETHYL-, ETHYL ESTER, (Z,E,E,E)-/CN              |
| E7      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,3,6-TRI          |
|         |     | METHYLPHENYL) $-3$ , $7$ -DIMETHYL-, ETHYL ESTER, $(Z, E, E, Z)$ -/CN |
| E8      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-FLUORO-9-(4-METHOXY-2,5-DIMET          |
|         | •   | HYL-1,3-CYCLOHEXADIEN-1-YL)-3,7-DIMETHYL-, ETHYL ESTER, (ALL          |
|         |     | -E) -/CN  |
| E9      | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-METHOXY-9-PHENYL-, ETHYL ESTE          |
|         |     | R/CN  |
| E10     | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-METHYL-9-PHENYL-, METHYL ESTE          |
|         |     | R, (2E, 4E, 6E, 8E) -/CN  |
| E11     | 1   | 2,4,6,8-NONATETRAENOIC ACID, 2-METHYL-9-PHENYL-, METHYL ESTE          |
|         |     | R, $(ALL-E)-/CN$  |
| E12     | 1   | 2,4,6,8-NONATETRAENOIC ACID, 3,7-DIETHYL-9-(2-(HEXYLOXY)PHEN          |
|         |     | YL)-, $(ALL-E)-/CN$   |
|         |     |   |
| => e3   |     | ·   |

L3 1 "2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, ETHYL ESTER"/CN

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ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
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84654-95-5 REGISTRY RN

ED Entered STN: 16 Nov 1984

CN 2,4,6,8-Nonatetraenoic acid, 2-cyano-9-phenyl-, ethyl ester (6CI, 9CI) (CA INDEX NAME)

3D CONCORD FS

C18 H17 N O2 MF

LCSTN Files: BEILSTEIN\*, CA, CAOLD, CAPLUS

(\*File contains numerically searchable property data)

# \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

- 4 REFERENCES IN FILE CA (1907 TO DATE)

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                  FBIB ----- AN, BIB, plus Patent FAM
                  IND ----- Indexing data
                  IPC ----- International Patent Classifications
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                  OIBIB ----- OBIB, indented with text labels
                                                                           t terms
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                                        containing hit terms
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#### => d 14 1-4 ti fbib abs

- ANSWER 1 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
- TI 1H and 13C NMR spectra and structure of some polyenic compounds
- 1995:915821 CAPLUS AN
- DN 124:74476
- 1H and 13C NMR spectra and structure of some polyenic compounds ΤI
- AU Kurkovskaja, L. N.; Genkina, N. K.; Shugol, V. L.
- Inst. Pishchevykh Veshchestv, Russia CS
- SO Zhurnal Strukturnoi Khimii (1995), 36(4), 703-8 CODEN: ZSTKAI; ISSN: 0136-7463
- PB Nauka
- DT Journal
- Russian LA
- The proton and 13C NMR spectra were determined of a series of Ph(CH:CH)nCH:CXY AΒ (X, Y are acceptor substituents). The proton-proton spin-spin interactions were used to determine the degrees of charge transfer in the CH:CH and CH-CH chains. The effects of substituents and chain length on this charge transfer are discussed.

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- L4 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN
- TI من Differential pulse polarography on bifurcate conjugate systems. المنافقة المن Homologous progressive change of the peak potential
- the things with 1986:5348 in CAPLUS to for a series of the transfer of the tenth of the tenth of the transfer of the tenth of the tenth of the transfer of the tenth of the te
  - DN 104:5348
- TI Differential pulse polarography on bifurcate conjugate systems. I. Homologous progressive change of the peak potential

  AU Hu, Weixiao; Yan, Baozhen; Tai, Tsuichen

  - Inst. Chem., Acad. Sin., Beijing, Peop. Rep. China CS
- CODEN: FKYYDG
  - DT Journal
  - LΑ Chinese
  - The polarog. reduction of the title class compds. [Ph(CH:CH)nCH:C(CN)2 (n =  $\frac{1}{2}$ ) 0-3), Ph(CH:CH)nCH:CAc2 (n = 0-3), Ph(CH:CH)nCH:C(CO2Et)2 (n = 0,1,3,5), Ph(CH:CH)nCH:C(CN)CO2Et (n = 0,1,3,5)] have two clear reduction waves, the peak potentials of which give LFER with (1/2)2/N. LFER are also observed between the HMO-calculated LUMO and the UV of the compds. within each series. LFER do not exist for peak potentials vs. LUMO for compds. in different units.
  - ANSWER 3 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN 1.4
  - Structural effect in branched conjugated systems bifurcation-type of TI branched polyenic nitriles, carboxylic acids and esters
  - ΑN 1983:88685 CAPLUS
  - DN 98:88685
  - Structural effect in branched conjugated systems bifurcation-type of TI branched polyenic nitriles, carboxylic acids and esters
  - AU Dai, Cuichen; Yu, Zhenjie; Jiang, Mingqian
  - Inst. Chem., Acad. Sin., Beijing, Peop. Rep. China CS
  - SO Scientia Sinica, Series B: Chemical, Biological, Agricultural, Medical & Earth Sciences (English Edition) (1982), 25(10), 1021-34 CODEN: SSBSEF; ISSN: 0253-5823
  - DT Journal
  - English LА
  - AB The UV spectra and NMR chemical shifts of the homologous series Me (CH:CH) nCH:C(CN) CO2Et (n = 0, 1, 3, 5), Ph(CH:CH) nCH:C(CN) R (n = 0, 1, 2, 3, 5; R = CN, CO2Et), and Ph(CH:CH)nCH:CR2 (R = CO2H, n = 1, 3, 5; R = CO2H) CO2Et, n = 0, 1, 3, 5) conformed to the rule of homologous linearity. In all of these branched compds., a red shift in the UV spectra was observed upon introduction of electron-attracting branching groups. Mass spectra

indicate that CN groups are more strongly conjugated with the polyenic chain than are CO2Et groups. Substituent effects of branching groups were calculated by the method of similar triangles.

L4ANSWER 4 OF 4 CAPLUS COPYRIGHT 2006 ACS on STN ΤI Vinylene "shift" in asymmetric phenylpolyenes AN 1957:29795 CAPLUS 51:29795 DN OREF 51:5739i,5740a-i,5741a Vinylene "shift" in asymmetric phenylpolyenes ΤI Wizinger, R.; Sontag, H. ΑU Univ. Basel, Switz. CS SO Helvetica Chimica Acta (1955), 38, 363-72 CODEN: HCACAV; ISSN: 0018-019X DΤ Journal LΑ German GI For diagram(s), see printed CA Issue. AΒ In the PhCH:CH(CH:CH)nPh series the bathochromic shift decreases in value from 28 mm with each integral increase in the value of n. The A second that is bathochromic effect ("shift") of the introduction of the 1st vinylene and the second that is a second to the second that is a second to the group and the convergence of the series has been investigated for the series RR'C:CH(CH:CH)nPh (I) where R is a chromophore group and R' is a series series as the series of the series either a chromophore group, H, or a group capable of ring-formation with R. I was synthesized by condensation of compds. containing a reactive Me. or was synthesized by condensation of compds. :CH2 group with m-phenylpolyene aldehydes prepared according to ாக அது அது அது Schmitt (C.A. 36, 65235) ap to 11-phenylundecapentaenal. ாhe coupling அவருக்கு அது அது அது இரு compds. were limited to passive components on account of poor yields with the higher aldehydes. Heating oxothianaphthene 30 min. in alc. containing few drops of piperidine with Ph(CH:CH)2CHO (II), Ph (CH:CH)3CHO (III), and Ph (CH:CH) 5CHO (IV) gave condensation products S.C6H4.CO.C:CH (CH:CH) nPh (A) (n, m.p., color of solution in alc. or AcOH, and  $\lambda$  in m $\mu$  given): 2, 153°; golden yellow, 469; 3, 170°, bright red, 482; 5, 212-13°, wine-red, 508. Similarly, condensation of 0.5 g. rhodanine (V) by heating 1 hr. on a steam bath with 0.9 g. II in 5 cc. 90% alc. containing 1.5 g. H2SO4, and condensation of 0.35 g. III with 0.25 g. V in 1 cc. Ac2O containing 3 drops piperidine under the same conditions yielded S.CS.NH.CO.C:CH(CH:CH)nPh (A'): 2, 218-19°, golden-yellow, 424; 3, 237-9°, orange, 449. AcPh in hot alc. in the presence of 3 drops 10% NaOH condensed with III and IV to produce BzCH:CH(CH:CH)nPh (B): 3, 120°, greenish yellow, 401; 5, 172-3°, golden-yellow, 429. Refluxing the analogous pyrylium salts of Series J in hot alc. 2 hrs. with excess aqueous MeNH2 gave [CH:CPh.CH:CPh.NMe.CCH:CH(CH:CH)nPh]ClO4 (C): 2, -, golden yellow, 420; 3, -, orange, 444; 5, -, red, 483. N-Methylquinaldinium Me sulfate (VI) (0.5 g.) was condensed by heating 1 hr. on a steam bath with 0.3 g. BzH in 1 cc. Ac20 containing 0.5 cc. pyridine, the product taken up in alc. and, after 2 hrs., treated with 5 cc. 20% NaClO4. This and similar condensations with PhCH: CHCHO, II, III, and IV gave [CH:CH.C6H4.NMe.CCH:CH(CH:CH)nPh]ClO4 (D): O, -, bright yellow, 379; 1, 225-7°, golden-yellow, 417; 2, 227°, orange, 483; 5, 278-80° (decomposition), red, 515. Condensation of 2methylbenzoselenazole ethiodide with BzH, PhCH:CHCHO, II and III by heating 1 hr. on a steam bath in alc. containing a few drops piperidine and treating the product with 20% aqueous NaClO4 gave [Se.C6H4.NEt.CCH:CH(CH:CH)nPh]ClO4(E):0,237-8°, golden yellow, 384; 1, 219-20°, orange, 426; 2, 198-200°, red-orange, 462; 3, above 190° (decomposition), red, 488. Condensations with NCCH2CO2Et gave EtO2C(CN)C:CH(CH:CH)nPh (F): 2, 166-7°, golden-yellow, 428; 3, 169°, red-orange, 465; 4, 190°, red, 497; 5, 210°, wine-red, 508. Condensations with barbituric acid and 5-methyl-2-phenyl-3-pyrazolone gave CO.NH.CO.NH.CO.C:CH(CH:CH)nPh (G): 3, 241-3°, red, 451; 5, 252-4°, blue-red, 503; and CMe:N.NPh.CO.C:CH(CH:CH)nPh (H): 2, 167°, orange, 409; 3,

163-4°, red, 449; 5, 197°, wine-red, 495. Similar

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condensation of 4,6-diphenyl-2-methylpyrylium sulfoacetate (cf. Schneider, C.A. 16, 1247) and conversion of the condensation products with 20% aqueous NaClO4 yielded [O.CPh:CH.CPh:CHCCH:CH(CH:CH)nPh]ClO4 (J): 2, 252-5° (decomposition), red-violet, 546; 3, 255° (decomposition), blue, 585; 5, above 250° (decomposition), green, 652. From tabulated values it is seen that the combined bathochromic effect for 5 vinylene groups varies from 76 mm in series A to 194 mm in series J, and that the introduction of the 1st vinylene group gives shifts ranging from 24 to 48 mu. With the exception of series A and A' there is a generally definite convergence of shift values due to increase of the number of vinylene linkages very similar to those noted in the diphenylpolyene series though much greater in series J and very dissimilar in E. Between the initial ultraviolet maximum and the shifts following the introduction of the 1st and of the combined groups no parallel behavior is apparent. The low average shift in series A and A' is indicative of a fundamental constitutional difference between these compds. and those of other series where the 1st C atom of the conjugated chain is linked with a chromophore system and an H atom or with two chromophores. Other problems of interest for future investigation are proposed.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information

on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> e1

L5 1 "2,4,6,8-NONATETRAENOIC ACID, 2-CYANO-9-PHENYL-, (ALL-E)-"/CN

=> d 15

L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

RN 81620-82-8 REGISTRY

ED Entered STN: 16 Nov 1984

CN 2,4,6,8-Nonatetraenoic acid, 2-cyano-9-phenyl-, (all-E)- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C16 H13 N O2

LC STN Files: BEILSTEIN\*, CA, CAPLUS, CASREACT (\*File contains numerically searchable property data)

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and the specific Double bond geometry as shown. The second sections of the second section of the second sec

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

1 REFERENCES IN FILE CA (1907 TO DATE)

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                                                   Structural effect in cross conjugative systems. IV. Properties of
                                   ΤI
                                                   a-carboxyphenylpolyenic cyanides and the quantum chemical
                                                   calculation of orbital energy and bond order
                                   AN
                                                   1982:180289 CAPLUS
                                   DN
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                                                   Structural effect in cross conjugative systems. IV. Properties of
                                                   α-carboxyphenylpolyenic cyanides and the quantum chemical
                                                   calculation of orbital energy and bond order
                            AU Liang, Desheng; Lai, Chugen; Chiang, Mingchien
     CS __Inst._Chem., Acad. Sin., Shanghai, Peop. Rep. China
                                  SO Fenzi Kexue Xuebao (1981-1982) (1981), 1(1), 17-30
   A COUNTY OF THE CODEN: FKXUDX; ISSN: 0253-3677 When the contraction of the contraction of
                                  DT Journal
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                               AB
                                                  all-trans-Ph(CH:CH)nCH:C(CN)CO2H (I) are prepared and their UV and mass
 ு அது differences, and π-bond orders அது கொடிக்கு இரு வரிக்கு வரிக்க
     of I are calculated by CNDO/2. The properties of I are correctly calculated by
                          using the extended form of the homologous equation for the corresponding
linear conjugated system (m-phenylpolyenic nitriles) with an
c-CO2H group substituent. Cross-conjugated systems may be generally treated by allowing 1 of the 2 branches to become the terminal group of a
 linear conjugated system while the other branch becomes the substituent.
      => d 16 it
                                  L6
                                                  ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
             . . . . . . . . . IT-

    Conjugation

                                                             (cross-, in α-carboxy(phenyl)polyolefinic nitriles, MO calcns.
                                                        and)
                                   IT
                                                  Molecular orbital
                                                             (for cross-conjugated α-carboxy(phenyl)polyolefinic nitriles)
                                   IT
                                                   Resonance
                                                             (in α-carboxy(ω-phenyl)polyolefinic nitriles)
                                   IT
                                                  Mass spectra
                                                             (of α-carboxy(ω-phenyl)polyolefinic nitriles)
                                   IT
                                                   Homologous series
                                                             (of \alpha-carboxy(\omega-phenyl)polyolefinic nitriles and related
                                                             linear conjugated systems, MO calcn. of)
                                   ΙT
                                                   Ultraviolet and visible spectra
                                                             (of \alpha-carboxy(\omega-phenyl)polyolefinic nitriles, MO calcn.
                                                             and)
                                   TT
                                                   Bond order
                                                             (poly-, in cross-conjugated α-carboxy(phenyl)polyolefinic
                                                             nitriles and related linear conjugated systems)
                                   IT
                                                   Stabilization energy
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                                                             nitriles)
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                                                   Carboxyl group
                                                              (\alpha-, effect of, on bond order and UV of \omega-
                                                             phenylpolyolefinic nitriles)
                                   IT
                                                   Nitriles, properties
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(\alpha-carboxy substituted \infty-phenylpolyenic, MO calcns. of)
                                                                 Unsaturated compounds
                                              IT
                                                                  RL: PRP (Properties)
                                                                               (cross-conjugated, MO calcn. of UV and other properties of)
                                                                  Energy level excitation
                                              IT
                                                                               (electronic, of \alpha-carboxy(\omega-phenyl)polyolefinic nitriles
                                                                              and related linear conjugated systems, MO calcn. of)
                                                                  100-47-0, properties
                                              IT
                                                                  RL: PRP (Properties)
                                                                               (UV of, MO calcn. of)
                                                                   65-85-0, properties 93-58-3 98-86-2, properties 100-52-7, properties
                                              IT
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                                                                  81620-81-7P 81620-82-8P 81620-83-9P
                                                                 RL: SPN (Synthetic preparation); PREP (Preparation)
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                                                                  10576-63-3P 28010-12-0P 53649-66-4P
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L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

IT 81620-82-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and UV and bond order of, MO calcn. of)

RN 81620-82-8 CAPLUS

CN 2,4,6,8-Nonatetraenoic acid, 2-cyano-9-phenyl-, (all-E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

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STRUCTURE FILE UPDATES: 10 APR 2006 HIGHEST RN 879997-63-4 DICTIONARY FILE UPDATES: 10 APR 2006 HIGHEST RN 879997-63-4

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http://www.cas.org/ONLINE/UG/regprops.html

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chain nodes

chain bonds:

exact/norm bonds :

1-2 2-3 2-6

Gl:O,N,Cl,Br,F,I,Cb

Match level :

1:CLASS 2:CLASS 3:Atom 6:CLASS

Generic attributes :

2:

Type of chain

: Linear

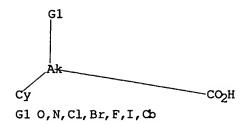
Saturation

: Unsaturated

Element Count: Node 2: Limited C,C5-6

L11 STRUCTURE UPLOADED

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Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SCREEN SEARCH COMPLETED - 154635 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS ( 2 INCOMPLETE) 5 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

FULL FILE PROJECTIONS: ONLINE SANTA \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: 3069536 TO 3115864 PROJECTED ANSWERS: 6552 TO 8910

L12 5 SEA SSS SAM L11

=> d scan

L12 5 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN Prostan-1-oic acid, 6,11,15-trihydroxy-9-oxo-, (6S,11 $\alpha$ ,15S)- (9CI)

MF C20 H36 O6

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):5

L12 5 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN 1H-Pyrrole-1-heptanoic acid, 2,3-bis(4-fluorophenyl)-β,δdihydroxy-5-(1-methylethyl)-4-[[[(4-methylphenyl)sulfonyl]amino]carbonyl], (βR,δR)- (9CI)

MF C34 H36 F2 N2 O7 S

Absolute stereochemistry.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L12 -5 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 3-Hexenoic acid, 5-[[(1,1-dimethylethoxy)carbonyl]amino]-6-phenyl-,

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organisation (3E, 5S) - (9CI) come of propositional and the control of the contro

MF С17 Н23 N О4

Absolute stereochemistry.

Double bond geometry as shown.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L12 5 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[3-(4-fluorophenyl)-1-(1-methylethyl)-4-phenyl-5-[[(2-pyridinylmethyl)amino]carbonyl]-1H-pyrrol-2-yl]-3,5-dihydroxy-, (3R,5S,6E)- (9CI)

MF C33 H34 F N3 O5

Absolute stereochemistry.

Double bond geometry as shown.

#### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L12 5 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[5-(4-fluorophenyl)-3-methyl-6-phenyl-4-pyridazinyl]-

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ير بريد بين monosodium salt, [R-[R\*,S\*-(E)]]- (9CI) بريد في من من المعالم الم

MF C24 H23 F N2 O4 . Na

Absolute stereochemistry.

Topics with Double bond geometry as shown. The same of the contraction of the contraction

Na

#### ALL ANSWERS HAVE BEEN SCANNED

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=> e 3-Hexenoic acid, 5-amino-6-phenyl/cn
                   3-HEXENOIC ACID, 5-AMINO-4-FLUORO-6-PHENYL-, (3E,5S)-/CN
E1
                   3-HEXENOIC ACID, 5-AMINO-4-FLUORO-6-PHENYL-, (3Z,5S)-/CN
E2
E3
             0 --> 3-HEXENOIC ACID, 5-AMINO-6-PHENYL/CN
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-/CN
F.4
E5
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5S)-, TRIFLUOROACETA
                   TE/CN
E6
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (S-(Z))-/CN
E7
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (S-(Z))-, TRIFLUOROACETA
E8
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, HYDROCHLORIDE, (S-(E))-/
E9
             1
                   3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, METHYL ESTER, (S-(E))-/C
E10
             1
                   3-HEXENOIC ACID, 5-BROMO-2-METHOXY-, ETHYL ESTER/CN
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3-HEXENOIC ACID, 5-CHLORO-/CN E11

3-HEXENOIC ACID, 5-CHLORO-, ETHYL ESTER, (E)-/CN E12

=> e4

L13 1 "3-HEXENOIC ACID, 5-AMINO-6-PHENYL-, (3E,5s)-"/CN

=> d 113

ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN L13

RN 521064-20-0 REGISTRY

ED Entered STN: 27 May 2003

CN 3-Hexenoic acid, 5-amino-6-phenyl-, (3E,5S)- (9CI) (CA INDEX

FS STEREOSEARCH

MF C12 H15 N O2

CI COM

SR CA

LC STN Files: CA, CAPLUS

<u> Balthara (1868) at 1964 at 1965 at 1966 at 1</u> <sub>。我们还是</sub>Absolute stereochemistry。 Rotation (+)。<sub>我们还是</sub>不是是一个人的人们的,我们也是一个人们的人们的人们的人们的人们 Double bond geometry as shown.

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L14 1 L13

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- L14 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
- TI Design and synthesis of amide isosteres of Phe-Gly: potential peptidomimetic ligands for the intestinal oligopeptide transporter PepT1
- AN 2002:692505 CAPLUS
- DN 138:354217
- TI Design and synthesis of amide isosteres of Phe-Gly: potential peptidomimetic ligands for the intestinal oligopeptide transporter PepT1
- AU Vabeno, Jon; Brisander, Magnus; Chen, Weiqing; Borchardt, Ronald T.; Luthman, Kristina
- CS Department of Medicinal Chemistry, University of Tromso, Tromso, N-9037, Norway
- SO Peptides: The Wave of the Future, Proceedings of the Second International and the Seventeenth American Peptide Symposium, San Diego, CA, United States, June 9-14, 2001 (2001), 610-611. Editor(s): Lebl, Michal; Houghten, Richard A. Publisher: American Peptide Society, San Diego, Calif.
  - CODEN: 69DBAL; ISBN: 0-9715560-0-8
- DT Conference

LA English

AΒ A symposium report. The transport of di- and tripeptides across the intestinal epithelium is an active process mediated by the oligopeptide transporter PepT1. Synthetic Phe-Gly peptidomimetics, where amide bond was replaced by isosteric moieties, were used in preliminary transport studies on Caco-2 cells.

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L16 1 L15

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- L16 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN
- Mode of addition to conjugated unsaturated systems. VI. Addition of halogens and hydrogen halides to conjugated unsaturated carboxylic acids and esters
- ΑN 1934:16632 CAPLUS
- DN 28:16632
- OREF 28:1984h-i,1985a-e
- Mode of addition to conjugated unsaturated systems. VI. Addition of halogens and hydrogen halides to conjugated unsaturated carboxylic acids
- Ingold, C. K.; Pritchard, G. J.; Smith, H. G. AU
- Journal of the Chemical Society (1934) 79-86 SO CODEN: JCSOA9; ISSN: 0368-1769
- DΤ Journal
- LΑ Unavailable
- cf. C. A. 27, 4775.  $\beta$ -Vinylacrylic acid- (I) and Cl in H2O give 60% AB of  $\delta$ -chloro- $\gamma$ -hydroxy- $\Delta\alpha$ -pentenoic acid (II), m. 73-4°; its structure was established by the action of 03, giving Accho, identified as the 2,4-dinitrophenylhydrazone, m. 299-300° property of the second secon (decomposition). I in Et2O, treated with aqueous HClO, gives a ം പ്രത്യാക്ക് dichlorodihydroxyvaleric acid, m. 166°ു പ and Clain H2O or I in ചെട്ടുക്കും ക്രൂക്കും ക്രൂക്കും Et20 and aqueous HBrO give the  $\delta$ -Br derivative corresponding to II, m. 92-3°. The addition of Br to sorbic acid in CS2 gives as the main product the crystalline  $\gamma, \delta$ -dibromide (III), together with a liquid byproduct, the quantity of which was considerable in CS2, CHC13 and hexane was supply but was much less in AcOH or with quinolinium tribromide in AcOH, all expts. at room temperature III with O3 gives MeCH: CBrCHO and CHOCO2H. The

The state of the dibromide contains III and some α, β-isomer. ICl and sorbic acid give γ-chloro-δ-iodo-β-ethýlacrylic acid (IV), m. followed by esterification, gives Et sorbate and Et  $\gamma$ -chlorosorbate, b15 105-10°, m. 31-2°. The action of Cl on sorbic acid in H2O or of aqueous HClO in Et2O gives 70% of  $\delta$ -chloro- $\gamma$ -hydroxy- $\Delta\alpha$ -hexenoic acid (V), m. 97°; oxidation with O3 gives ethylglyoxal, identified as the 2,4-dinitrophenylhydrazone, m. 247°; in neutral solution KMnO4 gives MeCHClCO2H; reduction of V with Pt oxide and H2 gives  $\delta$ -chloro- $\gamma$ -hexolactone, b16 130-2°, b756 243°, m. about 10°. The main product of the action of Br was the  $\delta$ -Br derivative corresponding to V, m. 110°; the oily byproduct, esterified with MeOH, gave a fraction analyzing for Me bromohydroxyhexenoate, b0.5 118°, and a fraction, C7H11O4Br, b0.5 148-50°, m. 154-5°. Me sorbate with Br in H2O gives Me  $\gamma$ ,  $\delta$ -dibromo- $\Delta\alpha$ -hexanoate, since 03 yields a-bromocrotonaldehyde, whose 2,4-dinitrophenylhydrazone, deep red, m. 220° (decomposition). Br and sorbic acid in EtOH give the  $\gamma$ -Br derivative, also obtained by the action of EtOH-KOH on the di-Br acid. 2,4-dinitrophenylhydrazone of AcH exists in 2 forms, the less stable modification, orange-red, m. 146°, changing to the more stable, yellow, m. 162°, on crystallization from EtOH. Liquid HCl and sorbic acid at room temperature for several days give an oil, which decomps. on distillation

and

consists largely of  $\delta$ -chloro- $\Delta\beta$ -hexenoic acid, since O3 gives AcCHO. Br and Et muconate give a dibromide, m. 81°, yielding with 03 Et  $\beta$ -bromo- $\beta$ -aldehydoacrylate, the 2,4dinitrophenylhydrazone of which, yellow, m. 193-4°, (CO2H)2 and (CHBrCO2H)2; ICl gives a compound, m. 68°, believed to be Et  $\beta$ -chloro- $\alpha$ -iodo- $\Delta\gamma$ -dihydromuconate.

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| FULL ESTIMATED COST                        | ENTRY<br>5.50  | SESSION<br>87.28 |
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### > e1

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L18 0 L17

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NEWS
                                  2
                                                       "Ask CAS" for self-help around the clock
                                                       New IPC8 SEARCH, DISPLAY, and SELECT fields in USPATFULL/
                      NEWS 3 DEC 23
                                                       USPAT2
                                        JAN 13
                                                       IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
                      NEWS 4
                                        JAN 13 New IPC 8 SEARCH, DISPLAY, and SELECT enhancements added to
                      NEWS 5
                                                       INPADOC
                      NEWS 6
                                     JAN 17
                                                       Pre-1988 INPI data added to MARPAT
                      NEWS 7 JAN 17
                                                       IPC 8 in the WPI family of databases including WPIFV
                                                       Saved answer limit increased
                      NEWS 8 JAN 30
                      NEWS 9 FEB 21 STN AnaVist, Version 1.1, lets you share your STN AnaVist
                                                       visualization results
                      NEWS 10 FEB 22 The IPC thesaurus added to additional patent databases on STN
                      NEWS 11 FEB 22 Updates in EPFULL; IPC 8 enhancements added
                      NEWS 12 FEB 27 New STN AnaVist pricing effective March 1, 2006
                      NEWS 13 FEB 28 MEDLINE/LMEDLINE reload improves functionality
                      NEWS 14 FEB 28 TOXCENTER reloaded with enhancements
                      NEWS 15 FEB 28 REGISTRY/ZREGISTRY enhanced with more experimental spectral
                                                       property data
                      NEWS 16 MAR 01 INSPEC reloaded and enhanced ...
             NEWS 17 MAR 03 Updates in PATDPA; addition of IPC 8 data without attributes
                      NEWS 18 MAR 08 X.25 communication option no longer available after June 2006
     Market is now updated on a daily-basis - was a second of the second of t
                      NEWS 20 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL
                      NEWS 21 APR 03 Bibliographic data updates resume; new IPC 8 fields and IPC
                                                       thesaurus added in PCTFULL
NEWS 23 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced
  NEWS #24 --- NEWS #24 --- APR -12 -- Improved structure highlighting in FQHIT and QHIT display
                                                       in MARPAT
NEWS 25 APR 12 Derwent World Patents Index to be reloaded and enhanced during
                                                       second quarter; strategies may be affected
```

NEWS EXPRESS FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a,
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AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005.
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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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\*\*\*\*\*\*\*\*\*

\* The CA roles and document type information have been removed from \*

\* the IDE default display format and the ED field has been added, \*

\* effective March 20, 2005. A new display format, IDERL, is now \*

\* available and contains the CA role and document type information. \*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

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REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

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COST IN U.S. DOLLARS
SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST
0.44
0.65

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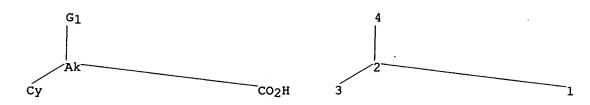
=>

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chain nodes : 1 2 3 4 chain bonds : 1-2 2-3 2-4 exact/norm bonds : 1-2 2-3 2-4

G1:0,N

-Match level: 1:CLASS 2:CLASS 3:Atom 4:CLASS

Generic attributes : a series a significant and a series and a series

2:

Type of chain

: Linear

Saturation

: Unsaturated

Element Count:

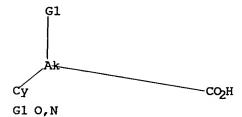
Node 2: Limited

L1STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam SAMPLE SEARCH INITIATED 05:37:53 FILE 'REGISTRY' SAMPLE SCREEN SEARCH COMPLETED - 149950 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*

9 ANSWERS

BATCH \*\*INCOMPLETE\*\*

PROJECTED ITERATIONS: PROJECTED ANSWERS:

2976177 TO 3021823

11937 TO 15053

L2

9 SEA SSS SAM L1

=> d scan

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 3,5-dihydroxy-7-phenyl-, [R-[R\*,S\*-(E)]]- (9CI)

MF C13 H16 O4

Absolute stereochemistry.

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):9

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN
IN 2-Pentenoic acid, 5-(1-cyclopenten-1-yl)-3-ethoxy-5-hydroxy- (9CI)
MF C12 H18 04

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\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[2-(3-chlorophenyl)-4-(4-chlorophenyl)-6-(1-methylethyl)-5-pyrimidinyl]-3,5-dihydroxy-, monosodium salt (9CI)

MF C26 H26 C12 N2 O4 . Na

C1

OH

OH

OH

$$CH = CH - CH - CH_2 - CH - CH_2 - CO_2H$$

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[3-cyclopropyl-4-(4-fluorophenyl)-6-(1-methylethyl)-1-phenyl-1H-pyrazolo[3,4-b]pyridin-5-yl]-3,5-dihydroxy-, monosodium salt, (3R,5S,6E)-rel- (9CI)

MF C31 H32 F N3 O4 . Na

Relative stereochemistry.

Double bond geometry as shown.

O-Na

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[6-chloro-4-(4-fluorophenyl)-2-(1-methylethyl)-3-quinolinyl]-3,5-dihydroxy- (9CI)

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MF C25 H25 C1 F N O4

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CI COM

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 5-Hexenoic acid, 2-amino-5-fluoro-6-phenyl-, (2S,5Z)- (9CI)

MF C12 H14 F N O2

Absolute stereochemistry.
Double bond geometry as shown.

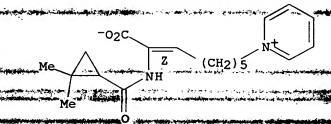
### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Pyridinium, 1-[7-carboxy-7-[(2,2-dimethylcyclopropyl)carbonyl]amino]-6heptenyl]-, inner salt, (Z)- (9CI)

MF C19 H26 N2 O3

Double bond geometry as shown.



L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[2-(4-fluorophenyl)-4,5,6,7-tetrahydro-7-(2-phenylethyl)-2H-indazol-3-yl]-3,5-dihydroxy-, monosodium salt, [3(3R\*,5S\*,6E),7R\*]- (9CI)

MF C28 H31 F N2 O4 . Na

Relative stereochemistry.
Double bond geometry as shown.

Na

L2 9 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN 6-Heptenoic acid, 7-[1-(4-fluorophenyl)-3-(1-methylethyl)-2-naphthalenyl]-3,5-dihydroxy-, monosodium salt, [R\*,S\*-(E)]- (9CI)

MF C26 H27 F O4 . Na

Relative stereochemistry.

Double bond geometry as shown.

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### ALL ANSWERS HAVE BEEN SCANNED

=> logoff hold

COST IN U.S. DOLLARS

ENTRY SESSION

FULL ESTIMATED COST

2.64

2.85

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FULL ESTIMATED COST
2.64
2.85

=> d his

L1

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FILE 'REGISTRY' ENTERED AT 05:32:11 ON 13 APR 2006 STRUCTURE UPLOADED

L2 9 SEARCH L1 SSS SAM

=> e 7-phenyl-2,4,6-heptatrienoic acid/cn E1 1 7-PHENYL-2,3-DICHLORODIBENZO-P-DIOXIN/CN

```
E2
                                                                                                                             7-PHENYL-2,4,6-HEPTATRIENAL/CN
                                                 E3
                                                                                                             1 --> 7-PHENYL-2,4,6-HEPTATRIENOIC ACID/CN
                                                                                                                      7-PHENYL-2,4,6-HEPTATRIENOYLHYDROXAMIC ACID/CN
7-PHENYL-2,5-NORBORNADIENE/CN
7-PHENYL-2-ANILINO-1-PHENYL-1,6-NAPHTHYRIDIN-4(1H)-ONE/CN
7-PHENYL-2-ANILINO-1-PHENYL-1,8-NAPHTHYRIDIN-4(1H)-ONE/CN
                                                 E4
                                                 E5
                                                 E6
                                                 E7
                                                                                                                                7-PHENYL-2-HEPTANONE/CN
                                                 E8
                                                                                                                                  7-PHENYL-2-NAPHTHALENOL/CN
                                                 E9
                                                 E10
                                                                                                                                  7-PHENYL-2-NAPHTHOL/CN
                                                                                                                                   7-PHENYL-2-OCTANONE/CN
                                                E11
                                                                                                        1
                                                 E12
                                                                                                                                        7-PHENYL-2-OXA-7-AZABICYCLO(3.2.0)HEPTAN-6-ONE/CN
                                                => e3
                                                                                                             1 "7-PHENYL-2,4,6-HEPTATRIENOIC ACID"/CN
                                                L3
                                                => d 13
                                                                       ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
                                                L3
                                               RN 6460-62-4 REGISTRY
ED Entered STN: 16 Nov 1984
                                                CN 2,4,6-Heptatrienoic acid, 7-phenyl- (7CI, 8CI, 9CI) (CA INDEX NAME)
entremported the Cother NAMES: "The proportion of the control of t
                                                CN 6-Phenyl-1,3,5-hexadiene-1-carboxylic acid
                                                 CN
                                                                       7-Phenyl-2,4,6-heptatrienoic acid
                                                                       Phenylbutadieneacrylic acid
         a traj ne je open JPS i rega 3D concord a<del>namentalia kinadani kandani </del>
                  MF C13 H12 O2
     LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMLIST, TOXCENTER,
USPAT2, USPATFULL
(*File contains numerically searchable property data)
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Ph-CH=CH-CH=CH-CO2H

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- 2 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
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FULL ESTIMATED COST

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        => 13
        L4
                    17 L3
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        APPS ----- AI, PRAI
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CLASS ----- IPC, NCL, ECLA, FTERM

DALL ----- ALL, delimited (end of each field identified)

DMAX ----- MAX, delimited for post-processing

FAM ----- AN, PI and PRAI in table, plus Patent Family data

FBIB ----- AN, BIB, plus Patent FAM

IND ----- Indexing data
        IPC ----- International Patent Classifications
        MAX ----- ALL, plus Patent FAM, RE
        PATS ----- PI, SO
        SAM ----- CC, SX, TI, ST, IT
        SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;
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                    SCAN must be entered on the same line as the DISPLAY,
        STD ---- BIB, CLASS
        IABS ----- ABS, indented with text labels
        IALL ----- ALL, indented with text labels
        IBIB ----- BIB, indented with text labels
        IMAX ----- MAX, indented with text labels
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        OIBIB ----- OBIB, indented with text labels
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        SIBIB ----- IBIB, no citations
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        HITRN ----- HIT RN and its text modification
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        HITSEQ ----- HIT RN, its text modification, its CA index name, its
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        FHITSTR ---- First HIT RN, its text modification, its CA index name, and
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FBIB ----- AN, BIB, plus Patent FAM

IND ----- Indexing data
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SAM ----- CC, SX, TI, ST, IT
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          PATS ----- PI, SO
                         e.g., D SCAN or DISPLAY SCAN)
           STD ----- BIB, CLASS
           IABS ----- ABS, indented with text labels
           IALL ----- ALL, indented with text labels
           IBIB ----- BIB, indented with text labels
           IMAX ----- MAX, indented with text labels
           ISTD ----- STD, indented with text labels
           OBIB ----- AN, plus Bibliographic Data (original)
           OIBIB ----- OBIB, indented with text labels
           SBIB ----- BIB, no citations
           SIBIB ----- IBIB, no citations
           HIT ----- Fields containing hit terms
           HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)
                        containing hit terms
           HITRN ----- HIT RN and its text modification
           HITSTR ----- HIT RN, its text modification, its CA index name, and
                        its structure diagram
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HITSEQ ----- HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields

FHITSTR ---- First HIT RN, its text modification, its CA index name, and its structure diagram

FHITSEQ ---- First HIT RN, its text modification, its CA index name, its structure diagram, plus NTE and SEQ fields

KWIC ----- Hit term plus 20 words on either side

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# => d 14 12-17 ti fbib abs

- L4 ANSWER 12 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
  - TI Synthesis of 5-aryl-2,4-pentadienals and 5-aryl-2,4,6-heptatrienoic acids
  - AN 1970:434990 CAPLUS
  - DN 73:34990
- TI Synthesis of 5-aryl-2,4-pentadienals and 5-aryl-2,4,6-heptatrienoic acids
  - AU Dombrovskii, A. V.; Pribytkova, L. G.; Ganushchak, N. I.; Vengrzhanovskii,
- CS Chernigov. Gos. Univ., Chernigov, USSR

  SO Zhurnal Organicheskoi Khimii (1970), 6(5), 964-7

  CODEN: ZORKAE; ISSN: 0514-7492

  DT Journal

  LA Russian

  - The reaction in the cold of XC6H4CH: CHCH: CH2 with POCl3HCONMe2 mixture in tetrahydrofuran gave 30-67% XC6H4CH:CHCH:CHCHO (I, X = H, p-Me, p-MeO, o-Cl, or p-Cl). The reaction of I with (EtO)2P(O)CHNaCO2Et gave 61-96% XC6H4CH:CHCH:CHCO2Et which was saponified to the corresponding acid.
  - L4
  - ANSWER 13 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

    (+)-(5S)-\delta-Lactone of 5-hydroxy-7-phenylhepta-2,6-dienoic acid, a ΤI natural product from Cryptocarya caloneura
  - AN 1968:29406 CAPLUS
  - DN 68:29406
  - ΤI  $(+)-(5S)-\delta$ -Lactone of 5-hydroxy-7-phenylhepta-2,6-dienoic acid, a natural product from Cryptocarya caloneura
  - ΑU Hlubucek, J. R.; Robertson, Alexander V.
  - CS Univ. Sydney, Sydney, Australia
  - SO Australian Journal of Chemistry (1967), 20(10), 2199-206 CODEN: AJCHAS; ISSN: 0004-9425
  - DΤ Journal
  - LA English
  - GI For diagram(s), see printed CA Issue.
  - AB The structure, including absolute configuration, of a new compound extracted from C.

caloneura was determined by degradation as the  $(+)-(5S)-\delta$ -lactone of 5-hydroxy-7-phenylhepta-2,6-dienoic acid (I). The structure was confirmed by synthesis of its racemate.

- L4ANSWER 14 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
- ΤI Reactions with phosphinealkylenes. VIII. Novel synthesis of carboxylic acids from phosphine alkylenes
- 1964:440194 CAPLUS AN
- 61:40194 DN

OREF 61:6945g-h,6946a-d Reactions with phosphinealkylenes. VIII. Novel synthesis of carboxylic acids from phosphine alkylenes ΑU Bestmann, Hans Juergen; Schulz, Heinz Tech. Hochschule, Munich, Germany CS Ann. (1964), 674, 11-17 SO DT Journal Unavailable LΑ cf. CA 59, 10111b. Phosphine alkylenes react with chlorocarbonates by AB transylidation to yield carbalkoxylated derivs. which can be used in various ways for the synthesis of carboxylic acids. Ph3P:CHCH:CH2 (I) reacted with ClCO2Me (II) in the  $\gamma$ -position to the P atom. A simple spot test for Ph3P is described. All reactions were performed under N. NaNH2 from 0.5 g. Na in about 100 cc. liquid NH3 treated. with 22 millimoles appropriate [RCH2PPh3]Cl (III), the NH3 evaporated, the residue refluxed 10 min. with 100 cc. dry C6H6, treated dropwise with 0.01 mole suitable chloroformate in 50 cc. dry C6H6, and filtered from the III (80-100%), and the residue from the filtrate recrystd. yielded the corresponding R(R'O2C)C:PPh3 (IV). In this manner were prepared the following IV (R' = Me) (R, m.p., and % yield given): H, 164° (AcOEt), 80; Me, 145° (AcOEt), 95; Et, 125° (AcOEt-petr. ether), 88; Pr (V), 105° (C6H6-petr. ether), 96; Ph (VI), 155° (AcOEt), 80; cyclohexyl, -(oil),75. VI (1.00 g.) and 10 cc. 20% KOH in 1:1 MeOHH2O refluxed 2 hrs., filtered from Ph3PO, and acidified with 2N H2SO4 yielded 0.32 g. PhCH2CO2H, m. 76°. The yield from 17.4-g. hexahydrobenzyltriphenylphosphonium bromide treated with 2.16 g. ClCO2Et and the oily product saponified gave 1.9 g. cyclohexylacetic acid, b3 110-15°, m. 30°. [PrPPh3]Br (8.8 g.) converted to the yield, treated with II, and filtered, the filtrate refluxed 10 hrs. with 1.06 g.

BzH, and the product refluxed 2 hrs. with 40 cc. KOH in 1:1 H20-MeOH

yielded 1.25 g. trans-PhcH:CEtCO2H, m. 105-6° (aqueous AcOH). V (2.00 g.) and 0.56 cc. BzH in 100 cc. dry AcOEt refluxed 8 hrs. yielded 0.78 g. trans-PhCH:CPrCO2H, needles, m. 93°. V (2.26 g.) and 0.71 cc. PhCH: CHCHO in 120 cc. dry AcOEt refluxed 24 hrs. gave similarly 0.87 g. PhCH:CHCH:CPrCO2H, needles, m. 145-6° (aqueous AcOH). PH3P:CMeCO2Et (21.7 g.) in C6H6 refluxed 2 hrs. with 6.0 g. BzCH2Br, filtered, concentrated to half-volume, refluxed 2 hrs. with 20 cc. Mel, filtered from 10.2 g. [MePPh3] I, and distilled gave 3.6 g. BzCH:CMeCO2Et, b0.4 160-5°; 2,4-dinitrophenylhydrazone, red, m. 149-50° (MeOH or AcOEt). [Ph3PCH2CH:CH2]Br (8.8 g.) converted to I, treated with 0.77 g. II, decanted from the oily precipitate, and evaporated, and the red oily product refluxed 2 hrs. with 50 cc. 2N NaOH in 1: 1 H20-MeOH gave 0.32 g. MeCH:CHCO2H, m. 71°; dicyclohexylamine salt m. 127°. The oily salt from a similar run refluxed 20 hrs. with 0.71 cc. BzH and refluxed 20 hrs. and worked up in the usual manner yielded 0.25 g. PhCH:CHCH:CHCO2H, m. 136-40°. A similar run with 1.32 g. PhCH:CHCHO during 10 hrs. gave 0.57 g. Ph(CH:CH) 3CO2H, m.  $189-90^{\circ}$  (becoming clear at  $198^{\circ}$ ); also obtained in 50% yield from PH3P:CHCH:CHCO2Me with PhCH:CHCHO. Ph3P with p-O2NC6H4CH2Cl yields [p-O2NC6H4CH2PPh3]Cl which is converted by alkali to the deep red, stable p-O2NC6H4CH:PPh3. A 2% solution of p-O2NC6H4CH2Cl in C6H6 applied to filter paper, a few drops of the solution

the presence of Ph3P.

L4 ANSWER 15 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN

TI Relation between the antimicrobial action and chemical structure of aromatic fatty acid. XI

to be tested for Ph3P added, and the paper heated at 100-20° for a

few min. and then treated with a drop of dilute aqueous NaOH gave a red color

AN 1963:430451 CAPLUS

DN 59:30451

in

OREF 59:5535g-h Relation between the antimicrobial action and chemical structure of aromatic fatty acid. XI ΑU Takechi, Kazutake CS Univ. Tokushima, Japan SO Hakko Kogaku Zasshi (1961), 39, 534-41 CODEN: HKZAA2; ISSN: 0367-5963 DT Journal Unavailable LA cf. CA 58, 11721c. Phenylpentadienylidenemalonic acid, AB phenylhexatrienecarboxylic acid, and pentachlorocinnamic acid (I) were prepared and their antimicrobial activities against yeasts, molds, and bacteria studied. The increase both in the number of conjugated double bonds and in that of C atoms of a fatty acid group attached to the phenyl radical enhanced the strength of antimicrobial action. As was reported previously (CA 55, 10374i) a monobasic acid was more effective than a dibasic acid. The activity of I was especially marked against all microorganisms studied. L4 ANSWER 16 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN Light absorption and double bonds TI AN 1934:25254 CAPLUS DN 28:25254 OREF 28:2999e-i,3000a-c TI Light absorption and double bonds imparing profession for AU made Hausser, in K. «W. . in 1998 in the color of page from a complete month of the AU made Hausser, in the color of the SO Zeitschrift fuer Technische Physik (1934), 15, 10-20 CODEN: ZTPHAU; ISSN: 0373-0093 Journal LA Unavailable

GI For diagram(s), see printed CA Issue. AB The absorption spectra of compds. containing conjugated double bonds are given for the region 750-200 mm (mol. absorption coefficient plotted against frequency): Me(CH:CH)nCO2H(n = 1,2,3,4) in absolute alc. (and for n = 4 at  $-190^{\circ}$  as well as at room temperature), Ph(CH:CH)nCO2H (n = 1,2,3), O-CH:CH:CH:C(CH:CH)nCO2H (n = 0,1,2,3,4), Ph(CH:CH)nPh (n = 1,2,3,4,5,6,7) in C6H6 at room temperature and at -190°, crocetin, carotene, lutein, zeaxanthin, physalien, taraxanthin, violaxanthin, carotene, lutein, zeaxanthin, physalien, taraxanthin, violaxanthin, methylbixin, lycopene and the indolenine dyes (n = 0,1,2,3). The fluorescence emission spectra of the diphenylpolyenes and the Raman spectra of Me(CH:CH)nCO2H (n = 1, 2, 3, 4, 5) and their mono-(n') and di-Me(n'') derivs. in EtOH, BuOH or CCl4 are also given. The strongest absorption band increases in intensity and is shifted to the longer wave lengths with increasing number of double bonds (n). The dependence of the position of the band on n is shown by the simple curve obtained by plotting the maximum frequency (corr. for solvent action) against n plus the color equivs. of the other chromophors in the compound (cf. C. A. 24, 343). Isolated double bonds appear to have no effect. All but the ionizable compds. (indolenine dyes, cyanidin chloride and polyenes in concentrated H2SO4) are of the same spectral type and show a cleavage of the band at the maximum which appears more clearly the larger n is, the lower the temperature, or the more sym. the mol. The fluorescence emission spectra are almost mirror images of the absorption spectra, but according to Stokes' law are displaced to the smaller frequencies. This frequency difference is brought about by the loss of energy by absorption and emission and by a solvent effect. The emission spectra of diphenyloctatetraene in various solvents are practically the same but the absorption spectra vary

considerably. The cleavage in both emission and absorption is controlled by the frequency (about 1600 cm.-1) of the C double bond. This frequency is also obtained from the Raman spectra. The principle Raman lines are for n = 1, 1655; 2, 1644; 2', 1639; 3, 1618; 3', 1608; 3'', 1601; 4, 1599; 5, 1576 cm.-1. This decrease with increase of n shows that the conjugated double bonds form a simple system which acts as a whole optically as well

as chemical The intensity of the Raman lines increases strongly with increase in n for similar concns.

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L4 ANSWER 17 OF 17 CAPLUS COPYRIGHT 2006 ACS on STN
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TI 7-Phenylhaptatrienic acid

AN 1929:31251 CAPLUS

DN 23:31251

OREF 23:3688f-i,3689a-d

TI 7-Phenylhaptatrienic acid

AU Vorlander, D.; Daehn, Erich

SO Ber. (1929), 62B, 545-9

DT Journal

LA Unavailable

AB cf. preceding abstract The study of 7-phenylheptatrienic acid (1) was of interest from the point of view of the behavior of the 3 double bonds in addition reactions and of the question whether crystalline-liquid (c.-1.)

are strengthened by lengthening the chain even without p-substitution.

Unlike the aldehyde, I can be obtained pure and was shown to be enantiotropic c.-1. There is thus now available the series BzOH, PhCH:CHCO2H, PhCH:CHCO2H and I in which the c.-1. properties increase with the lengthening of the chain and introduction of each further CH:CH group, although it does not establish whether the C:C groups act only spatially by lengthening the chain, or also energetically, or, which is most probable, cumulatively through several very different functions. The بين معهنت معهنية yield of phenylpentadienalmalonic acid was increased from 40 to 60% by معمنية معهنية منافعة المعمنية والمعالية والمعالية والمعالية المعالية المعالي using aic, NH3 instead of AcOH in the, condensation; it seps. from alc. in orange needles, m. about 191° (m. ps. corrected) with evolution of CO2 (Erlenmever and Engelberg, 190°; V., Fischer and Kunze, 210-2°). With 2 parts Ac20 at 120-30° it gives about 30% I, almost colorless or yellowish white, gives a yellow-brown color with and NH4 salts, microcryst, ppts. I and its Na salt in H2O suspension are strikingly stable toward light, even ultra-violet, only a small part decomposing In CHCl3 I adds 3 mols. Br2 without appreciable evolution of HBr. Me ester, prepd, with MeOH and H2SO4, very faintly yellowish, m. 114°, non-c.-1., gives a brown color with H2SO4; Et ester, almost colorless, m. 91, non-c.-1, (a mixture of the Me and Et esters is likewise non-c.-1.), can be supercooled and then solidifies rhythmically with marked contraction; this crystalline-solid phase changes on standing into 2 crystalline-solid phases. Chloride, prepared with SOC12, brownish mass. Anilide, dull yellow, m. 213°, forms 2 crystalline-solid phases, non-c.-1., gives a red-brown color with H2SO4. p-Toluide, pale yellow, m. 209°, faint monotropic c.-1. schlicren, gives a red-brown color with H2SO4. p-Aniside, yellow- green, dimorphous enantiotropic c.-1., m. 203-4° (presumably transition solid  $\rightarrow$  c.-1.), gives a red-brown color with H2SO4. p-Phenclide, yellow-greenish, m. 210-1°, enantiotropic c.-1., then 3amorphous-liquid; like the aniside, on cooling there appear a 1st and a 2nd crystalline-liquid phase.

With

Na-Hg and CO2 in H2O on the H2O bath, I gives a di- or tetrahydro derivative, waxy leaflets, m.  $64^{\circ}$ , gives a brown color with H2SO4, reduces KMnO4, is non-c.-1., becomes yellowish and sticky after 2-3 days in the air and light. The C content lies between the values caled, for C13H14O2 and C13H16O2 and the H content is too low for the latter formula but titration with Br in CHCls points to a tetrahydro acid with only one C:C bond. There are no definite relations between the light and color phenomena under a quartz ultra-violet lamp and the degree of unsatn. of the compds. p-MeOC6H4CHBrCHBrCHBrCO2H shines with an unusually bright pink color, anisic acid glows at least as strongly as p-MeOC6H4CH:CHCO2H or the Me ester of I, but BzOH more weakly than PhCH:CHCO2H. The phenomenon changes with shifting of the double bond from p-MeOC6H4CH3CH:CHCH2CO2H (faintly luminous) to the  $\alpha$ ,  $\beta$ -unsatd.

isomer (strongly luminous) or on rearrangement of MeOC6H4CH:CHCH:CHCO2H (strongly luminous) into the allo-acid (weakly luminous). Complete hydrogenation usually, but apparently not always, decreases the luminescence. All the arylideneamines hitherto tested appear black in the light of the quartz Hg lamp, as does Et p-azoxycinnainate, whereas phenylhydrazones glow brightly and the anilides, anisides, etc., of the acids are more or less bright.

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```
=> e 6-Heptenoic acid, 3,5-dihydroxy-7-phenyl-, [R-[R*,S*-(E)]]-/cn
                     1 6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-(TRIBUTYLSTANNYL)-, BUTYL
ESTER, (3R,5R,6E)-/CN
ESTER, (3R, 5R, 6E) -/CN
E2 1 6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-(TRIBUTYLSTANNYL)-, METHYL
ESTER/CN
E3
                  0 --> 6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, R-R*,S*-(E)-/
          E4
                       1
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, (R*,S*-(E))-/CN
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, (R^*, S^*-(E))-(\pm
          E5
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, (R-(R*,S*-(E)))-/
          E7
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 1,1-DIMETHYLETHYL
                             ESTER/CN
          E8
                       1
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 1,1-DIMETHYLETHYL
                             ESTER, (3R, 5S, 6E) - /CN
          E9
                       1
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 1,1-DIMETHYLETHYL
                              ESTER, (R^*, S^*)-/CN
          E10
                       1
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 1,1-DIMETHYLETHYL
                              ESTER, (R^*, S^*) - (\pm) - /CN
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 1,1-DIMETHYLETHYL
          E11
                       1
                             ESTER, (S-(R^*, S^*-(E)))-/CN
          E12
                             6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, 4,7,7-TRIMETHYL-3
                             - (1-NAPHTHALENYL) BICYCLO(2.2.1) HEPT-2-YL ESTER/CN
          => e4
          L5
                       1 "6-HEPTENOIC ACID, 3,5-DIHYDROXY-7-PHENYL-, (R*,S*-(E))-"/CN
          => d 15
          L5
               ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN
          RN
               121308-01-8 REGISTRY
          ED
               Entered STN: 23 Jun 1989
               6-Heptenoic acid, 3,5-dihydroxy-7-phenyl-, [R*,S*-(E)]- (9CI)
               (CA INDEX NAME)
          OTHER CA INDEX NAMES:
```

6-Heptenoic acid, 3,5-dihydroxy-7-phenyl-,  $[R^*,S^*-(E)]-(\pm)$ -CN

FS STEREOSEARCH

MF C13 H16 O4

SR CA

LC STN Files: BEILSTEIN\*, CA, CAPLUS

(\*File contains numerically searchable property data)

Relative stereochemistry. Double bond geometry as shown.

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=> 15

L6

1 L5

=> d 16 ti fbib abs

ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN L6

ΤI QSAR study of the role of hydrophobicity in the activity of HMGR

inhibitors 1989:417158 CAPLUS AN DN 111:17158 ΤI QSAR study of the role of hydrophobicity in the activity of HMGR ΑU Prabhakar, Yenamadra S.; Saxena, Anil K.; Doss, M. Jinandra CS Med. Chem. Div., Cent. Drug Res. Inst., Lucknow, 226 001, India SO Drug Design and Delivery (1989), 4(2), 97-108 CODEN: DDDEEJ; ISSN: 0884-2884 DTJournal English LΑ AB The 3-hydroxy-3-methylglutaryl-CoA reductase (HMGR) inhibitory activity of 7-(aryl/biphenyl)-6-heptenoic acids was quant. analyzed by using hydrophobicity, van der Waals volume, and electronic parameters. activity was primarily a function of hydrophobicity, and was well correlated with the hydrophobicity of ortho and meta substituents on the aryl/biphenyl moiety. The electronic properties of para substituents on the aryl/biphenyl ring influenced the inhibition. Substituents with pos. polar and sigma and neg. resonance consts. might lead to better inhibition. => d 16 it ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN (of aryl or biphenylheptenoates) IT Hydrophobicity (of aryl or biphenylheptenoates, hydroxymethylglutarylCoA reductase inhibition and structure in relation to)

IT Molecular structure-property relationship (hydrophobicity, of aryl or biphenylheptenoates)

IT Molecular structure biological activity relationship

(hydroxymethylglutaryl CoA reductase-inhibiting, of aryl or biphenylheptenoates) IT Molecular structure-biological activity relationship (quant., of aryl or biphenylheptenoates)  $\cdot \cdot$  IT ecular structure-property relationship (resonance energy, of aryl or biphenylheptenoates) Molecular structure-property relationship IT Molar volume and Molecular volume (van der Waals, of aryl or biphenylheptenoates, hydroxymethylglutarylCoA reductase inhibition and structure in relation to) IT 7732-18-5 RL: BIOL (Biological study) (hydrophobicity, of aryl or biphenylheptenoates, hydroxymethylglutarylCoA reductase inhibition and structure in relation IT 108033-99-4 **121308-01-8** 121308-02-9 121308-03-0 121308-04-1 121308-05-2 121308-06-3 121308-07-4 121308-08-5 121308-09-6 121308-10-9 121308-11-0 121308-12-1 121308-13-2 121308-14-3 121308-15-4 121308-16-5 121308-17-6 121308-18-7 121308-19-8 121308-20-1 121308-21-2 121308-22-3 121308-23-4 121308-24-5 121308-25-6 121308-26-7 121308-27-8 121308-28-9 121308-29-0 121308-30-3 121308-31-4 121308-32-5 121308-33-6 121308-34-7 121308-35-8 121308-36-9 121308-37-0 121308-38-1 121308-39-2 121308-40-5 121308-41-6 121308-42-7 121308-43-8 121308-44-9 121308-45-0 121308-46-1 121308-47-2 121308-48-3 121308-49-4 121308-50-7 121308-51-8 121308-52-9 121308-53-0 121308-54-1 121308-55-2 121308-56-3 121308-57-4 121308-58-5 121308-59-6 121308-60-9 121308-61-0 121308-62-1 121308-63-2 121308-65-4 121308-66-5 121308-67-6 121308-64-3 121308-68-7

121308-70-1 121308-71-2 121308-72-3

121308-73-4

121308-69-8

121308-74-5 121322-31-4 121322-32-5 121322-33-6 121322-34-7 121322-35-8 121322-36-9 121322-37-0 121322-38-1 121328-10-7

123783-51-7

RL: BIOL (Biological study)

(hydroxymethylglutarylCoA reductase inhibition by, structure in relation to)

IT 9028-35-7, 3-Hydroxy-3-methylglutarylcoenzyme A reductase

RL: PROC (Process)

(inhibition of, by aryl or biphenylheptenoates, structure in relation

=> 121308-01-8

### REG1stRY INITIATED

Substance data SEARCH and crossover from CAS REGISTRY in progress... Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

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L8

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ENTER ANSWER NUMBER OR RANGE (1):1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2006 ACS on STN

121308-01-8

RL: BIOL (Biological study)

(hydroxymethylglutarylCoA reductase inhibition by, structure in relation to)

121308-01-8 CAPLUS

6-Heptenoic acid, 3,5-dihydroxy-7-phenyl-, [R\*,S\*-(E)]- (9CI) (CA INDEX

Relative stereochemistry. Double bond geometry as shown.

=> logoff hold

COST IN U.S. DOLLARS TOTAL SINCE FILE ENTRY SESSION FULL ESTIMATED COST 13.98 57.36

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE 0.00 -5.25

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| => file reg   | •  |  |
| COST IN U.S. DOLLARS  | SINCE FILE   | TOTAL                                      |
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| FULL ESTIMATED COST   | 14.44  | 57.82                                      |
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\* \* The CA roles and document type information have been removed from \* \* the IDE default display format and the ED field has been added, \* \* effective March 20, 2005. A new display format, IDERL, is now \* available and contains the CA role and document type information. \* \*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

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http://www.cas.org/ONLINE/UG/regprops.html

```
=> e 5-Hexenoic acid, 2-amino-5-fluoro-6-phenyl-, (2S,5Z)-/cn
                                                                         5-HEXENOIC ACID, 2-AMINO-5-CHLORO-4-HYDROXY-/CN
                    E1
                    E2
                                                              1
                                                                                 5-HEXENOIC ACID, 2-AMINO-5-FLUORO-6-PHENYL-, (2R,5Z)-/CN
                                                              1 --> 5-HEXENOIC ACID, 2-AMINO-5-FLUORO-6-PHENYL-, (2S,5Z)-/CN
                    E3
                                                                           5-HEXENOIC ACID, 2-AMINO-5-METHYL-, (S)-/CN
                    E4
                    E5
                                                                              5-HEXENOIC ACID, 2-AMINO-5-METHYL-, METHYL ESTER/CN
                    E6
                                                                               5-HEXENOIC ACID, 2-AMINO-5-METHYL-4-METHYLENE-/CN
                                                                                 5-HEXENOIC ACID, 2-AMINO-5-METHYL-4-METHYLENE-, METHYL ESTER
                    E7
                   E8
                                                                               5-HEXENOIC ACID, 2-AMINO-6,6-DICHLORO-4-METHYL-, (2S,4S)-/CN
                                                                                 5-HEXENOIC ACID, 2-AMINO-6-BORONO-, (2S,5E)-/CN
                   E9
                                                                                 5-HEXENOIC ACID, 2-AMINO-6-PHENYL-, (2S)-/CN
                    E10
                                                                                 5-HEXENOIC ACID, 2-AZIDO-4,5-DIMETHYL-, METHYL ESTER, (R*,R*
                    E11
                                                                                 ) -/CN
                                  5-HEXENOIC ACID, 2-AZIDO-4-METHYL-, METHYL ESTER, (R*,R*)-/C
                   E12
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=> e3 .

L9 1 "5-HEXENOIC ACID, 2-AMINO-5-FLUORO-6-PHENYL-, (2S,5Z)-"/CN

=> d 19

L9 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2006 ACS on STN

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RN 219924-46-6 REGISTRY

ED Entered STN: 23 Feb 1999

CN 5-Hexenoic acid, 2-amino-5-fluoro-6-phenyl-, (2S,5Z) (9CI) (CA INDEX NAME)

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FS STEREOSEARCH

MF C12 H14 F N O2

SR CA

LC STN Files: CA, CAPLUS, CASREACT

Absolute stereochemistry.

Double bond geometry as shown.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

| => file caplus                             |            |         |
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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 7.92 8.13

FULL ESTIMATED COST

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FILE 'REGISTRY' ENTERED AT 09:54:52 ON 13 APR 2006

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4 SEARCH L1 SSS SAM

E 2-CYANO-2,4,6-HEPTATRIENOIC ACID/CN

E HEPTATRIENOIC ACID/CN

E 7-PHENYL- 2-CYANO-2,4,6-HEPTATRIENOIC ACID/CN

E 7-PHENYL- 2-CYANOLOGOFF HOLD-2,4,6-HEPTATRIENOIC ACID/CN

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# => d scan 12

4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L2ITERATION INCOMPLETE

D-arabino-2-Octulosuronic acid, 5-O-[2-(acetylamino)-2-deoxy-β-D-IN glucopyranosyl]-3-deoxy-, (45)- (9CI)

C16 H25 N O13 MF

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

### HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L2

1,3-Benzenedicarboxylic acid, 5-[(3-carboxy-1-oxo-2-propenyl)amino]-, IN

1,3-bis(1-methylethyl) ester (9CI)

C18 H21 N O7 MF

### ALLES PROPERTY, DATA AVAILABLE IN THE PROP'S FORMAT \*\* CONTROL OF THE PROPERTY OF THE PROPERTY

4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2,5-bis[[[4-[[4-[(3-carboxy-1-oxo-2-

propenyl)amino]phenyl]sulfonyl]phenyl]amino]carbonyl]-, (Z,Z)- (9CI)

and the second of the second

MF C41 H30 N4 O14 S2

# Double bond geometry as shown.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

L2 4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN Neuraminic acid, 4-O-(3-methoxyphenyl)- (9CI)

Absolute stereochemistry.

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

### ALL ANSWERS HAVE BEEN SCANNED

=> d 11

L1 HAS NO ANSWERS

L1 STR

G1 O,N

G2 O, S, N

Structure attributes must be viewed using STN Express query preparation.

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9.24 9.45

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=> d 110 1-2 ti fbib abs

- LIO ANSWER 1 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
  TI Enhanced Diastereoselectivity in the Asymmetric Ugi Reaction Using a New TI Enhanced Diastereoselectivity in the Asymmetric Ugi Reaction Using a New "Convertible" Isonitrile. [Erratum to document cited in CA130:125373] AN 1999:624076 CAPLUS
  DN 132:12484

  - Enhanced Diastereoselectivity in the Asymmetric Ugi Reaction Using a New "Convertible" Isonitrile. [Erratum to document cited in CA130:125373]
  - ΑU Linderman, Russell J.; Binet, Sophie; Petrich, Samantha R.
  - CS Dept. Chem., North Carolina State Univ., Raleigh, NC, 27695-8204, USA
  - Journal of Organic Chemistry (1999), 64(21), 8058 CODEN: JOCEAH; ISSN: 0022-3263
  - PB American Chemical Society
  - DΤ Journal
  - English LA
  - AB On page 337, R for compds. 8b, 10b, and 11b in Table 1 and Scheme 3 should be CH2CH(CH3)2 rather than CH(CH3)2. The diastereoselectivities reported using isonitrile 1 with the arabinosyl auxiliary 9 are not significantly enhanced relative to those reported by Kunz and coworkers (reference 5b) using tert-Bu isocyanide at -78 °C. In addition, Kunz and Pfrengle (J. Am. Chemical Society 1988, 110, 651-652 and reference 5a) report an example of an asym.

Ugi reaction using phenylisonitrile that resulted in a 94:6 dr.

- L10 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2006 ACS on STN
- Enhanced Diastereoselectivity in the Asymmetric Ugi Reaction Using a New "Convertible" Isonitrile
- AN 1999:3600 CAPLUS
- DN 130:125373
- TI Enhanced Diastereoselectivity in the Asymmetric Ugi Reaction Using a New "Convertible" Isonitrile
- AU Linderman, Russell J.; Binet, Sophie; Petrich, Samantha R.
- CS Department of Chemistry, North Carolina State University, Raleigh, NC, 27695-8204, USA
- SO Journal of Organic Chemistry (1999), 64(2), 336-337

CODEN: JOCEAH; ISSN: 0022-3263

PB American Chemical Society

DT Journal

LA English

OS CASREACT 130:125373

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AB The authors report a new "convertible" isonitrile (I) which not only provides a means for milder hydrolysis of the amide product form a Ugi multicomponent condensation reaction, but results in improved diastereoselectivities of both (R)- and (S)-amino acids via the asym. Ugi reaction using the galactosylamine and arabinosylamine chiral auxiliaries II and III (Piv = Me3CCO) developed by H. Kunz, et al.; (1988, 1989). Thus, Ugi condensation of I with aldehyde PhCH:CFCH2CH2CHO, galactosylamine auxiliary II, and HCHO in the presence of ZnCl2 gave 65% of the corresponding adduct, which was treated with 2N HCl at 60° for 24 h to give 75% amino acid IV via desilylation, an amide to ester intramol. exchange, and hydrolysis.

RE.CNT 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

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NEWS 6
         JAN 17 Pre-1988 INPI data added to MARPAT
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                 INSPEC reloaded and enhanced
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         MAR 03
                 Updates in PATDPA; addition of IPC 8 data without attributes
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                 X.25 communication option no longer available after June 2006
NEWS 19 MAR 22 EMBASE is now updated on a daily basis
NEWS 20 APR 03 New IPC 8 fields and IPC thesaurus added to PATDPAFULL
                 Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
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         APR 03
                 Thesaurus added in PCTFULL
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NEWS 22 APR 04
NEWS 23 APR 12 LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 24 APR 12
                 Improved structure highlighting in FQHIT and QHIT display
                  in MARPAT
NEWS 25
         APR 12
                 Derwent World Patents Index to be reloaded and enhanced during
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| CARBAMFINDS/A  | TEMP        | 2 ANSWERS IN FILE CAPLUS     |
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        JAN 13 IPC 8 searching in IFIPAT, IFIUDB, and IFICDB
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        JAN 17 Pre-1988 INPI data added to MARPAT
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        JAN 17 IPC 8 in the WPI family of databases including WPIFV
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FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8 DICTIONARY FILE UPDATES: 11 APR 2006 HIGHEST RN 880129-32-8

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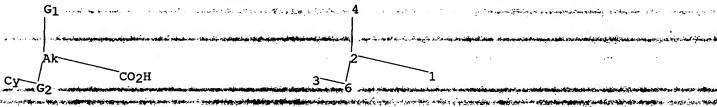
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chain nodes:
1 2 3 4 6
chain bonds:
1-2 2-4 2-6 3-6
exact/norm bonds:
1-2 2-4 2-6 3-6

G1:0,N

G2:0,S,N

Match level :

1:CLASS 2:CLASS 3:Atom 4:CLASS 6:CLASS

Generic attributes :

2:

Type of chain : Linear Saturation : Unsaturated

Element Count : Node 2: Limited C,C3-7

STRUCTURE UPLOADED

=> d 11 L1 HAS NO ANSWERS

Structure attributes must be viewed using STN Express query preparation.

=> search 11 sss sam
SAMPLE SEARCH INITIATED 09:59:43 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 149950 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS ( 2 INCOMPLETE) 4 ANSWERS INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

PROJECTED ITERATIONS: 2976177 TO 3021823 PROJECTED ANSWERS: 4959 TO 7037

L2 4 SEA SSS SAM LI

=> d scan

L2 4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN ITERATION INCOMPLETE

IN Neuraminic acid, 4-O-(3-methoxyphenyl)- (9CI)

MF C16 H23 N O9

Absolute stereochemistry.

\*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):4

L2 4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN

IN Benzoic acid, 2,5-bis[[[4-[[4-[(3-carboxy-1-oxo-2-propenyl)amino]phenyl]sulfonyl]phenyl]amino]carbonyl]-, (Z,Z)- (9CI)

MF C41 H30 N4 O14 S2

Double bond geometry as shown.

PAGE 1-E

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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IN 1,3-Benzenedicarboxylic acid, 5-[(3-carboxy-1-oxo-2-propenyl)amino]-,

1,3-bis(1-methylethyl) ester (9CI)

MF C18 H21 N O7

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

4 ANSWERS REGISTRY COPYRIGHT 2006 ACS on STN L2 ITERATION INCOMPLETE

IN D-arabino-2-Octulosuronic acid, 5-O-[2-(acetylamino)-2-deoxy-β-Dglucopyranosyl]-3-deoxy-,  $(4\xi)$ - (9CI)

C16 H25 N O13 MF

### \*\*PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT\*\*

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SESSION WILL BE HELD FOR 60 MINUTES STN INTERNATIONAL SESSION SUSPENDED AT 10:01:17 ON 13 APR 2006

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID: SSSPTA1623PAZ

COST IN U.S. DOLLARS

### PASSWORD:

\* \* \* \* \* \* RECONNECTED TO STN INTERNATIONAL \* \* \* \* \* SESSION RESUMED IN FILE 'REGISTRY' AT 10:07:36 ON 13 APR 2006 FILE 'REGISTRY' ENTERED AT 10:07:36 ON 13 APR 2006 COPYRIGHT (C) 2006 American Chemical Society (ACS)

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|                  |                                | ENTRY         | SESSION          |
| FULL ESTIMATED C | OST                            | 4.84          | 5.05             |
|                  |                                |               |                  |
| => e 2-cyano-2,4 | ,6-heptatrienoic acid/cn       |               |                  |
| E1 1             | 2-CYANO-2,3-DIMETHYLNONANOIC   | ACID 4-HYDROX | YPHENYL ESTER/CN |
| E2 1             | 2-CYANO-2, 3-DIMETHYLNONANOIC  |               |                  |
| E3 0 -           | -> 2-CYANO-2,4,6-HEPTATRIENOIC |               |                  |
| E4 1             | 2-CYANO-2,4-DIMETHYL-4-CYCLO   |               | ONE/CN           |
| E5 1             | 2-CYANO-2,4-DIMETHYL-5-P-MET   |               |                  |
|                  | ONE/CN                         |               |                  |

```
2-CYANO-2, 4-DIMETHYL-5-P-NITROPHENYL-4-CYCLOPENTENE-1, 3-DION
                       E6
                                                                      E/CN
                                                                      2-CYANO-2, 4-DIMETHYL-5-PHENYL-4-CYCLOPENTENE-1, 3-DIONE/CN
                       F.7
                                                       1
                                                                      2-CYANO-2, 4-DIPHENYL-4-CYCLOPENTENE-1, 3-DIONE/CN
                       E.8
                                                       1
                       E9
                                                       1
                                                                      2-CYANO-2-((2-METHYLPHENYL)AZO)ACETAMIDE/CN
                       E10
                                                                      2-CYANO-2-((2-METHYLPHENYL)HYDRAZONO)ACETAMIDE/CN
                       E11
                                                                      2-CYANO-2-((3-METHYLPHENYL)AZO)ACETAMIDE/CN
                       E12
                                                                      2-CYANO-2-((3-METHYLPHENYL)HYDRAZONO)ACETAMIDE/CN
                       => e heptatrienoic acid/cn
                                                                      HEPTATRIENE, METHYL-/CN
                                                       1
                       E2
                                                                     HEPTATRIENE, METHYL-, HOMOPOLYMER/CN
                       E3
                                                       0 --> HEPTATRIENOIC ACID/CN
                       E4
                                                      1
                                                                 HEPTATRIENONE/CN
                       E5
                                                      1
                                                                     HEPTATRIENYL ANION/CN
                       E6
                                                       1
                                                                    HEPTATRIENYL TRIANION/CN
                       E7
                                                                     HEPTATRIENYLIUM/CN
                                                                    HEPTATRIENYLIUM, 1,1'-(OXYDI-4,1-PHENYLENE)BIS(7-(4-METHOXYP
                                                                                                                                                              The company of the State of the
                                                                    HENYL) -/CN
                      E9 Company Transport 1 1 HEPTATRIENYLIUM, 1,1'-(OXYDI-4,1-PHENYLENE) BIS (7-(4-METHOXYP) (2014)
                                                                     HENYL) -, SULFATE (1:2)/CN
                       E10
                                                                     HEPTATRIENYLIUM, 1,1,7,7-TETRAKIS(4-(DIBUTYLAMINO)PHENYL)-/C
CHLORIDE/CN
E12 *** ** HEPTATRIENYLIUM, *1, 1, 7, 7-TETRAKIS (4- (DIETHYLAMINO) -2, 6-DIMET
                                                                      HOXYPHENYL) -/CN
                                                Martine, and any retirement receive miles or prices and an amendment appropriate applications and an expension of the contract of the contract
                            e 7-phenyl- 2-cyano-2,4,6-heptatrienoic acid/ch
                                                                     7-PHENOXYSULFONYL-3-INDENECARBOXYLIC ACID/CN
                                                                                                                                                                                                         m(t+k):=m+1.
                                                                      7-PHENOXYTRICYCLO(4.2.2.02,5) DEC-7-ENE-3,4,9,10-TETRACARBOXY
                                                                     LIC DIANHYDRIDE/CN
                      E3
                                                       0 --> 7-PHENYL- 2-CYANO-2,4,6-HEPTATRIENOIC ACID/CN
                      E4
                                                                      7-PHENYL-1,2,3,4-TETRAHYDROISOQUINOLINE/CN
                      E5
                                                                      7-PHENYL-1,2,3,4-TETRAHYDROQUINOLINE/CN
                                                       1
                      E6
                                                            7-PHENYL-1,2,4-TRIAZOLO(4,3-B)PYRIDAZINE/CN
                                                       1
                      E7
                                                      1
                                                                      7-PHENYL-1,2-NAPHTHALENEDICARBOXYLIC ANHYDRIDE/CN
                                                                      7-PHENYL-1,3,3-TRIMETHYLSPIRO(INDOLINE-2,3'-(3H)-NAPHTHO(2,1
                       E8
                                                       1
                                                                      -B) PYRAN) /CN
                                                       1
                       E9
                                                                      7-PHENYL-1,3,5-CYCLOHEPTATRIENE/CN
                       E10
                                                       1
                                                                      7-PHENYL-1, 3-DIAZASPIRO (4.4) NONANE-2, 4-DIONE/CN
                       E11
                                                                      7-PHENYL-1,4,6-ANDROSTATRIENE-3,17-DIONE/CN
                       E12
                                                                      7-PHENYL-1, 6-DIAZABICYCLO (4.1.0) HEPTANE/CN
                       => e 7-phenyl- 2-cyanologoff hold-2,4,6-heptatrienoic acid/cn
                       E1
                                                       1
                                                                      7-PHENOXYSULFONYL-3-INDENECARBOXYLIC ACID/CN
                       E2
                                                       1
                                                                      7-PHENOXYTRICYCLO(4.2.2.02,5)DEC-7-ENE-3,4,9,10-TETRACARBOXY
                                                                      LIC DIANHYDRIDE/CN
                       E3
                                                       0 --> 7-PHENYL- 2-CYANOLOGOFF HOLD-2,4,6-HEPTATRIENOIC ACID/CN
                      E4
                                                       1
                                                                    7-PHENYL-1,2,3,4-TETRAHYDROISOQUINOLINE/CN
                      E5
                                                       1
                                                                      7-PHENYL-1,2,3,4-TETRAHYDROQUINOLINE/CN
                       E6
                                                       1
                                                                      7-PHENYL-1, 2, 4-TRIAZOLO (4, 3-B) PYRIDAZINE/CN
                                                                      7-PHENYL-1, 2-NAPHTHALENEDICARBOXYLIC ANHYDRIDE/CN
                       E7
                                                       1
                       E8
                                                                      7-PHENYL-1,3,3-TRIMETHYLSPIRO(INDOLINE-2,3'-(3H)-NAPHTHO(2,1
                                                                      -B) PYRAN) /CN
                       E9
                                                       1
                                                                      7-PHENYL-1,3,5-CYCLOHEPTATRIENE/CN
                       E10
                                                       1
                                                                      7-PHENYL-1, 3-DIAZASPIRO (4.4) NONANE-2, 4-DIONE/CN
                       E11
                                                                      7-PHENYL-1, 4, 6-ANDROSTATRIENE-3, 17-DIONE/CN
                       E12
```

7-PHENYL-1,6-DIAZABICYCLO(4.1.0)HEPTANE/CN

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